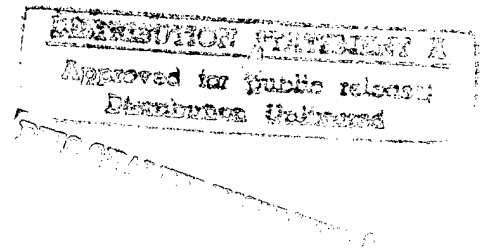Technical Report No. 8

VISCOSITY AND STRAIN GRADIENT EFFECTS ON

THE KINETICS OF PROPAGATING

PHASE BOUNDARIES IN SOLIDS

by

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Abstract

The theory of thermoelastic materials undergoing solid-solid phase transformations requires constitutive information that governs the evolution of a phase boundary. This is known as a *kinetic relation* which relates a *driving traction* to the speed of propagation of a phase boundary. The kinetic relation is prescribed in the theory from the onset. Here, though, a special kinetic relation is *derived* from an *augmented* theory that includes viscous, strain gradient and heat conduction effects. Based on a special class of solutions, namely traveling waves, the kinetic relation is inherited from the augmented theory as the viscosity, strain gradient and heat conductivity are removed by a suitable limit process.

1 Introduction

Materials can exist in different solid phases which are characterized, at a microscopic level, by their underlying crystalline structure. A change in temperature, stress or other variables can induce a material to change from one solid phase to another. Phase changes are usually classified according to the main mechanism driving the transformation, viz., by diffusion of chemical species or by displacement, although these are not mutually exclusive (see CHRISTIAN [8]). The present work deals with the latter type in which the transition from one phase to another is characterized by a sudden change in the crystalline lattice, achieved without diffusion but rather via a cooperative movement of atoms.

Inside a body, the interface between two distinct phases, known as a *phase boundary*, can be modeled as a surface of zero thickness across which the displacement is continuous but the deformation gradient suffers a jump. Other models, related to the Landau-Ginzburg theory, consider the interface as a transition layer of small but finite thickness where the deformation gradient varies rapidly but continuously (see, e.g., ERICKSEN [13], PENROSE & FIFE [21], TRUSKINOVSKY [27]). Implicit in the term "small" is the idea that the model has some kind of length scale. Some related theories that incorporate *separate* balance principles associated with the motion of material particles *and* the motion of the phase boundary have also been proposed (see, FRIED & GURTIN [15], LUSK [19]).

Within the framework of classical thermoelasticity theory, the thermomechanical properties of a material can be described by a Helmholtz free energy density that depends smoothly on the deformation gradient and the

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temperature. In order to model a material that can exist in different solid phases—and hence analyze phase transitions—the Helmholtz potential, at some temperatures, exhibits multiple wells. Each well is associated to a distinct solid phase. The nonconvexity of the potential allows the existence of weak solutions to dynamic problems. The solutions involve *shock waves*— across which the deformation gradient is discontinuous but the material on each side of the surface of discontinuity is in the *same* phase—and propagating phase boundaries if on each side the material phases are *different*.

Phase transformations in solids have been studied in recent papers by ABEYARATNE & KNOWLES [1, 3, 4, 5]. In particular, [5] deals with the *adiabatic* theory for a propagating phase boundary in a one-dimensional thermoelastic solid where an initial value problem of the Riemann type is analyzed. The phase boundary is modeled as a sharp interface. It is found that the solution to the Riemann problem is *not* unique. In order to recover uniqueness, Abeyaratne and Knowles propose the existence of an additional piece of constitutive information, a *kinetic relation*, which restricts the mobility of the phase boundary and singles out a unique solution for the Riemann problem. Following Onsager's formalism in thermodynamics (see, e.g., CALLEN [6], TRUESDELL [26]), the kinetic relation relates a *driving traction* (associated with a jump in entropy) to the speed of propagation of the phase boundary and to a state parameter, namely the temperature. In the sharp interface theory, the kinetic relation is introduced from the *onset*.

The purpose of the present analysis is to *derive* a special kinetic relation from an admissibility criterion related to a traveling wave problem in which an *augmented* theory is used. In the augmented (or *regularized*) theory, the

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sharp discontinuities are replaced by *transition layers* of finite thickness. By introducing dissipation and dispersion mechanisms associated with higher order derivatives of the strain (viscosity and strain gradient in this case), the phase boundary acquires a *structure*, i.e., it is possible to simulate a region where the strain varies rapidly but continuously. The augmented theory also includes heat conduction in order to have a continuously varying temperature across the transition layer. In a sense, the sharp interface theory should be obtained from the augmented theory through a suitable limit process where the dissipation and dispersion mechanisms and the heat conduction are removed.

In Section 2, the basic field equations and jump conditions are derived for the sharp interface theory and the results are specialized using a model for a thermoelastic material proposed in [3]. In Section 3, an augmented theory is introduced. Some general features of solutions to the traveling wave problem are derived in Section 4. It is also shown that the admissibility criterion for the existence of a subsonic traveling wave in the augmented theory provides an additional restriction on the data that can be cast as a kinetic relation.

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2 Sharp interface theory: adiabatic case

2.1 Basic equations.

Consider a bar that occupies the interval $[-L, L]$ in a reference configuration. Consider longitudinal motions of the bar during a time interval $[t_0, t_1]$. Points in the reference configuration are denoted by $(x, t) \in [-L, L] \times [t_0, t_1]$. Assume that the particle x is mapped to the position $y(x, t)$ at time t, (i.e., $y(x, t) = x + u(x, t)$, where u is the displacement); assume that $u \in C^0([-L, L] \times [t_0, t_1])$ and piecewise $C^2([-L, L] \times [t_0, t_1])$. Let $\gamma = u_x$ and $v = u_t$ be the strain and particle velocity (the subscript refers to partial differentiation). The restriction $-1 < \gamma(x, t)$, $\forall x, t$, guarantees that the deformation $y(x, t)$ is one-to-one. Let ρ be the *referential* mass density (assumed to be independent of x), σ the stress, ϵ the internal energy per unit mass and η the entropy. Assume that σ, ϵ and η are piecewise $C^1([-L, L] \times [t_0, t_1])$. The balance of linear momentum, balance of energy and the Clausius-Duhem inequality (dissipation inequality) for an *adiabatic thermomechanical process* in a one-dimensional bar are

$$[\sigma]_{x_1}^{x_2} = \frac{d}{dt} \int_{x_1}^{x_2} \rho v \, dx \ , \tag{1}$$

$$[\sigma v]_{x_1}^{x_2} = \frac{d}{dt} \int_{x_1}^{x_2} \rho \left(\epsilon + \frac{1}{2} v^2 \right) dx \ , \tag{2}$$

$$\Gamma(t) = \frac{d}{dt} \int_{x_1}^{x_2} \rho \eta \, dx \geq 0 \ , \tag{3}$$

$\forall t \in [t_0, t_1]$ and $\forall [x_1, x_2] \subseteq [-L, L]$. Here, $\Gamma(t)$ is the entropy production rate in the interval $[x_1, x_2]$. The local versions of (1), (2) and (3) at points where

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σ, v, γ, ϵ and η are smooth are

$$\sigma_x = \rho v_t \ , \tag{4}$$

$$(\sigma v)_x = \rho \left(\epsilon + \frac{1}{2} v^2 \right)_t \ , \tag{5}$$

$$\eta_t \geq 0 \ . \tag{6}$$

The compatibility equation is

$$v_x = \gamma_t \ . \tag{7}$$

Equation (5), with the use of (4), can be expressed as

$$\sigma \gamma_t = \rho \epsilon_t \ . \tag{8}$$

Let $x = s(t)$ be a point in $[x_1, x_2]$ across which some (or all) of the fields are discontinuous. Localization at $x = s(t)$ of the compatibility equation (7) and the global balances (1)-(3) provide the corresponding jump conditions, viz.,

$$[\![v]\!] + \dot{s}[\![\gamma]\!] = 0 \ , \tag{9}$$

$$[\![\sigma]\!] + \rho \dot{s}[\![v]\!] = 0 \ , \tag{10}$$

$$[\![\sigma v]\!] + \rho \dot{s}[\![\epsilon + \frac{1}{2} v^2]\!] = 0 \ , \tag{11}$$

$$[\![\eta]\!] \dot{s} \leq 0 \ , \tag{12}$$

where $\dot{s} = ds/dt$ is the speed of propagation of the discontinuity and, for any function g, $[\![g]\!] \equiv g^+ - g^-$ and $g^\pm = \lim_{x \to s(t)^\pm} g(x, t)$. The superscript

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refers to one side of the moving discontinuity as follows: the "+" ("−") side is the front (back) state if $\dot{s} > 0$ or the back (front) state if $\dot{s} < 0$. Moving discontinuities are said to be *compressive* if the strain in the front state is higher than in the back state and *expansive* otherwise. The velocity jump can be eliminated from (10) by using (9), i.e.,

$$[\![\sigma]\!] = \rho\dot{s}^2[\![\gamma]\!] \; . \tag{13}$$

Similarly, (11), with the use of (9) and (10), can also be expressed as

$$(\rho[\![\epsilon]\!] - \langle\sigma\rangle[\![\gamma]\!])\dot{s} = 0 \; , \tag{14}$$

where, for any function g, $\langle g \rangle \equiv (1/2)(g^+ + g^-)$.

2.2 Thermoelastic material.

A thermoelastic material can be characterized by its Helmholtz free energy, which is a function of strain and temperature, or by its internal energy, which is a function of strain and entropy. It can also be characterized by its Gibb's energy or by the enthalpy. One of these potentials is taken as a fundamental quantity and the others can be obtained from it via various Legendre transformations. If certain invertibility requirements between variables are met, it is possible to express these potentials in terms of any combination of two variables. If the strain and the temperature are used as variables, then the stress and the entropy are viewed as functions of γ and θ. As shown in subsequent sections, for the thermoelastic materials considered here—which are capable of phase transformations—the stress $\bar{\sigma}$ is *not* a monotonic function

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of γ or θ and the entropy $\bar{\eta}$ is *not* a monotonic function of γ. Nevertheless, it is assumed that the entropy is a monotonic function of the temperature, hence either (γ, θ) or (γ, η) can be used as variables. The following notation is employed: a function of strain and temperature is denoted as $\bar{g}$ and a function of strain and entropy is denoted as $\tilde{g}$. *Throughout the present analysis, the preferred variables are γ and θ.* Let the Helmholtz potential be given by $\psi = \bar{\psi}(\gamma, \theta)$. This potential is related to the internal energy through

$$\psi = \epsilon - \theta\eta . \tag{15}$$

For a classical thermoelastic material, the stress σ and the entropy η are given by

$$\sigma = \bar{\sigma}(\gamma, \theta) = \rho\bar{\psi}_\gamma(\gamma, \theta) , \tag{16}$$

$$\eta = \bar{\eta}(\gamma, \theta) = -\bar{\psi}_\theta(\gamma, \theta) . \tag{17}$$

The isothermal elastic modulus μ, the specific heat at constant strain c and the coefficient of thermal expansion α are defined by

$$\bar{\mu} = \rho\bar{\psi}_{\gamma\gamma} , \quad \bar{c} = -\theta\bar{\psi}_{\theta\theta} , \quad \bar{\alpha} = -\frac{\bar{\psi}_{\gamma\theta}}{\bar{\psi}_{\gamma\gamma}} . \tag{18}$$

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Alternatively, one can introduce the modified[1] Grüneisen coefficient defined, in terms of the above quantities, as

$$\bar{G} = \frac{\bar{\psi}_{\gamma\theta}}{\theta\bar{\psi}_{\theta\theta}} = \frac{\bar{\alpha}\bar{\mu}}{\rho\bar{c}} \ . \tag{19}$$

As a fundamental assumption, only materials with positive specific heat at constant strain and positive coefficient of thermal expansion are considered, i.e., $\forall(\gamma,\theta) \ \bar{c}(\gamma,\theta) > 0$. Hence, it is assumed that $\bar{G}(\gamma,\theta) \geq 0$. Moreover, since $\theta > 0$ and by $(18)_2$, then $\bar{\eta}$ is a strictly increasing function of θ. Thus, it is possible to define an inverse function $\theta = \tilde{\theta}(\gamma,\eta)$. The natural variables for the internal energy are γ and η. From equation (15), in terms of the Helmholtz potential, $\tilde{\epsilon}$ is given by

$$\tilde{\epsilon}(\gamma,\eta) = \bar{\psi}(\gamma,\tilde{\theta}(\gamma,\eta)) + \tilde{\theta}(\gamma,\eta)\eta \ . \tag{20}$$

Therefore, from (16) and (20), the stress can also be expressed as a function of γ and η, i.e., $\sigma = \tilde{\sigma}(\gamma,\eta) = \rho\tilde{\epsilon}_{\gamma}(\gamma,\eta)$. Similarly, the temperature is given by $\theta = \tilde{\theta}(\gamma,\eta) = \tilde{\epsilon}_{\eta}(\gamma,\eta)$. The isentropic elastic modulus μ_e is defined as $\bar{\mu}_e = \rho\tilde{\epsilon}_{\gamma\gamma}$. Henceforth, though, from the invertibility of η and θ, the internal energy ϵ is to be considered as given by a function $\bar{\epsilon}$ of γ and θ, i.e., $\epsilon = \bar{\epsilon}(\gamma,\theta) = \tilde{\epsilon}(\gamma,\bar{\eta}(\gamma,\theta))$. In terms of γ and θ, the isentropic elastic modulus μ_e can be expressed as

$$\bar{\mu}_e = \rho\left(\frac{\bar{\psi}_{\gamma\gamma}\bar{\psi}_{\theta\theta} - \bar{\psi}_{\gamma\theta}^2}{\bar{\psi}_{\theta\theta}}\right) \ . \tag{21}$$

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[1]The Grüneisen coefficient is usually defined as $(1+\gamma)G$, where G is given by (19). It turns out that (19) is a more convenient parameter. See CLIFTON [9].

The isothermal and the isentropic sound speeds, a and a_e, are defined, when $\mu, \mu_e > 0$, by

$$\bar{a} = \sqrt{\frac{\bar{\mu}}{\rho}} \, , \qquad \bar{a}_e = \sqrt{\frac{\bar{\mu}_e}{\rho}} \, . \tag{22}$$

Using the material parameters defined by (18), it follows from (21) and (22) that the sound speeds are related by

$$a_e^2 = a^2 \left(1 + \frac{\alpha^2 a^2}{c} \theta \right) \, ; \tag{23}$$

hence, if $\mu, \mu_e > 0$ and since $c > 0$, then $a_e^2 \geq a^2$. In the adiabatic theory, discontinuities are classified into two types, viz., *shock waves* and *phase boundaries*. Shock waves are related to a discontinuity where the material on each side is in the *same* phase. A phase boundary refers to the case where different material phases exist on each side of a propagating discontinuity. Moreover, a shock wave whose Lagrangian velocity $\dot{s}$ is zero is referred to as a *contact discontinuity* and a phase boundary with $\dot{s} = 0$ is called a *stationary phase boundary*.

Some authors define shock waves as traveling discontinuities that satisfy the so-called subsonic-supersonic condition *regardless* of the phases on each side of the discontinuity. The subsonic-supersonic condition asserts that $\dot{s}$ is bounded below by the isentropic sound speed of its front state and bounded above by the isentropic sound speed of its back state (see DUNN & FOS-DICK [11], TRUSKINOVSKY [27]). For a material with a nonconvex Helmholtz energy, it is possible to have moving discontinuities where the phases in the front and the back are different but the speed of propagation satisfies the

subsonic-supersonic condition. Here, though, those discontinuities will be referred to as *supersonic* phase boundaries. TRUSKINOVSKY [27] refers to *subsonic* phase boundaries as *kinks*. It will be shown that only subsonic phase boundaries have room for a kinetic relation.

2.3 Driving traction and kinetic relation.

Using (15)-(17) in (8) provides an alternative expression for the energy equation, i.e.,

$$\eta_t = 0 \ . \tag{24}$$

It follows that the dissipation inequality (6) is trivially satisfied at regular points. The rate of entropy production for a segment $[x_1, x_2]$ of the bar which contains a propagating discontinuity at $x = s(t)$ can be expressed as $\Gamma(t) = \Gamma_b(t) + \Gamma_s(t)$, where

$$\Gamma_b(t) = \int_{x_1}^{x_2} \rho \eta_t dx \ , \quad \Gamma_s(t) = -\rho[\![\eta]\!]\dot{s} \ . \tag{25}$$

Here, Γ_b represents the bulk entropy production and Γ_s corresponds to the entropy production due to the moving discontinuity. Equations (24) and $(25)_1$ imply that $\Gamma_b = 0$, hence the entropy production for a thermoelastic material under an adiabatic process occurs solely because of the presence of a moving discontinuity. Based on this entropy production, define the *driving traction* as

$$f = -\rho[\![\eta]\!]\langle\theta\rangle \ . \tag{26}$$

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For a discussion on the notion of driving traction, see ABEYARATNE & KNOWLES [1, 4] and TRUSKINOVSKY [27]. For a thermoelastic material, (14)-(17) and (26) provide the following equivalent expression for the driving traction when $\dot{s} \neq 0$

$$f = \rho \left\{ [\![\bar{\psi}]\!] - \langle \bar{\psi}_\gamma \rangle [\![\gamma]\!] - \langle \bar{\psi}_\theta \rangle [\![\theta]\!] \right\} . \tag{27}$$

In terms of the driving traction, the dissipation inequality (12) can be expressed as

$$f\dot{s} \geq 0 . \tag{28}$$

Therefore, the jump conditions are given by (9)-(12) or, equivalently, by (9), (13), (14) and (28). For given conditions on one side of the discontinuity, say (γ^+, θ^+), and for a given speed of propagation $\dot{s}$, the set of points (γ^-, θ^-) that satisfy the jump condition (13) is called the *Rayleigh set*. Similarly, for given conditions (γ^+, θ^+), the set of points (γ^-, θ^-) that satisfy the jump condition (14) is called the *Hugoniot set* (see DUNN & FOSDICK [11]). The *admissible* states (γ^+, θ^+) and (γ^-, θ^-) are those that belong to the Rayleigh *and* Hugoniot sets generated at either (γ^+, θ^+) or (γ^-, θ^-) and also satisfy the entropy jump condition (28). In problems of the Riemann type for bars made of thermoelastic materials that can undergo phase transformations, the jump conditions are not sufficient to fully determine the solution. Additional information is provided by the kinetic relation. Following Onsager's approach to irreversible thermodynamics, the quantity $f/\langle\theta\rangle$ is identified as an *affinity* and $\dot{s}$ as the corresponding *flux* (see ABEYARATNE & KNOWLES [1, 4]). The

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kinetic relation is part of the constitutive theory and relates the affinity to the flux and to a state parameter, in this case the temperature, i.e.,

$$\frac{f}{\langle\theta\rangle} = F(\dot{s}, \theta) , \tag{29}$$

where F is a *materially-determined* function.

2.4 A specific thermoelastic material.

In order to obtain results in specific problems, consider a thermoelastic material introduced by ABEYARATNE & KNOWLES [3]. A phase diagram of this material in the γ,θ-plane is shown in Figure 1. For temperatures below a critical temperature θ_C, the material can exist in either a low strain phase P_1 or a high strain phase P_3. These phases are metastable and are separated by an unstable phase P_2. Above the critical temperature the material can only exist in a stable phase P. Throughout this analysis, only transformations from or to the low and high strain phases are considered. A thorough description of the thermomechanical characteristics of this material can be found in [3]. The boundaries between the different phases are given by

$$\gamma_M(\theta) = \gamma_C + M(\theta - \theta_C) , \quad \gamma_m(\theta) = \gamma_C + m(\theta - \theta_C) , \tag{30}$$

where $\gamma_C > 0$, $\theta_C > 0$, M and m are constants. The expression for the Helmholtz potential is given in each phase by

$$\bar{\psi}(\gamma, \theta) = \begin{cases} \dfrac{\mu}{2\rho}\gamma^2 - \dfrac{\alpha\mu}{\rho}\gamma(\theta - \theta_T) - c\theta \log\left(\dfrac{\theta}{\theta_T}\right) & \text{in } P_1, \\[3ex] \dfrac{\mu}{2\rho}\left[\gamma^2 - \dfrac{\gamma_T(\gamma - \gamma_M)^2}{\gamma_m - \gamma_M}\right] \\ \quad - \dfrac{\alpha\mu}{\rho}\gamma(\theta - \theta_T) - c\theta \log\left(\dfrac{\theta}{\theta_T}\right) & \text{in } P_2, \\[3ex] \dfrac{\mu}{2\rho}(\gamma - \gamma_T)^2 - \dfrac{\alpha\mu}{\rho}(\gamma - \gamma_T)(\theta - \theta_T) \\ \quad - c\theta \log\left(\dfrac{\theta}{\theta_T}\right) + \dfrac{\lambda_T}{\theta_T}(\theta - \theta_T) & \text{in } P_3, \end{cases} \qquad (31)$$

where θ_T is the transformation temperature, γ_T is the transformation strain, λ_T is the latent heat at $\theta = \theta_T$ and $\gamma_m = \gamma_m(\theta)$, $\gamma_M = \gamma_M(\theta)$. The remaining parameters were defined in Section 2.2 and are assumed constant. It is convenient to introduce a set of nondimensional parameters defined as follows:

$$\left.\begin{aligned} T = \frac{c\theta}{a^2\gamma_T^2}, \quad & \delta = \frac{\gamma}{\gamma_T}, \quad \bar{v} = \frac{v}{a\gamma_T}, \\ l_T = \frac{\lambda_T}{a^2\gamma_T^2}, \quad & \mathsf{G} = G\gamma_T, \\ \mathsf{v} = \frac{\dot{s}}{a}, \quad \mathsf{M} = \frac{a^2\gamma_T M}{c}, \quad & \mathsf{m} = \frac{a^2\gamma_T m}{c}. \end{aligned}\right\} \qquad (32)$$

The variable δ might be viewed as a "normalized" strain. The parameter G will also be called the (modified) Grüneisen coefficient. Nondimensional

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internal energy **e**, stress τ and entropy **s** are defined as

$$\mathbf{e} = \frac{\epsilon}{a^2\gamma_T^2}, \quad \tau = \frac{\sigma}{\rho a^2\gamma_T}, \quad \mathbf{s} = \frac{\eta}{c}. \tag{33}$$

The nondimensional isentropic sound speed is $\mathbf{a_e} = a_e/a$, hence, from (23), it can be expressed as $\mathbf{a_e^2} = 1 + \mathbf{G}^2 T$. Other nondimensional parameters will be introduced as required. From (16) and (31), the stress response function is given by

$$\bar{\tau}(\delta, T) = \begin{cases} \delta - \mathbf{G}(T - T_T) & \text{low strain phase,} \\[2mm] \left[\delta - \dfrac{\delta - \delta_\mathsf{M}}{\delta_\mathsf{m} - \delta_\mathsf{M}}\right] - \mathbf{G}(T - T_T) & \text{unstable phase,} \\[2mm] (\delta - 1) - \mathbf{G}(T - T_T) & \text{high strain phase,} \end{cases} \tag{34}$$

where $\delta_\mathsf{m} = \delta_\mathsf{m}(T)$, $\delta_\mathsf{M} = \delta_\mathsf{M}(T)$. Observe that, for a fixed temperature, the stress-strain relation is linear in each phase. Hence, this material will be referred to as the *trilinear* material. The entropy response function, from (17) and (31), is given by

$$\bar{\mathbf{s}}(\delta, T) = \begin{cases} \mathbf{G}\delta + \left(1 + \log \dfrac{T}{T_T}\right) & \text{low strain phase,} \\[4mm] \begin{aligned} &\mathbf{G}\delta + \left(1 + \log \dfrac{T}{T_T}\right) \\ &\quad - \dfrac{1}{2(\mathsf{m} - \mathsf{M})}\left[\dfrac{(\delta - \delta_C)^2}{(T - T_C)^2} - \mathsf{M}^2\right] \end{aligned} & \text{unstable phase,} \\[4mm] \mathbf{G}(\delta - 1) + \left(1 + \log \dfrac{T}{T_T}\right) - \dfrac{l_T}{T_T} & \text{high strain phase.} \end{cases} \tag{35}$$

where the explicit forms of δ_m and δ_M given by (30) were used. The jump conditions for the special thermoelastic material when the high strain phase is on the *right* of the phase boundary (and the low strain phase on its left) are, from (13), (14), (28), (31), (34) and (35), given by

$$\left. \begin{array}{r} (1 - v^2)[\![\delta]\!] - 1 - G[\![T]\!] = 0 \; , \\[2mm] \left\{ G\langle T \rangle [\![\delta]\!] + [\![T]\!] - \left(\langle \delta \rangle - \dfrac{1}{2} \right) - GT_T - l_T \right\} v = 0 \; , \\[2mm] \left\{ G \left([\![\delta]\!] - 1 \right) + \log \dfrac{T^+}{T^-} - \dfrac{l_T}{T_T} \right\} v \leq 0 \; . \end{array} \right\} \qquad (36)$$

Similar expressions can be obtained when the low strain phase is on the right of the phase boundary. Using $(36)_1$ in $(36)_2$ to eliminate $[\![\delta]\!]$ gives

$$r_1(v)[\![T]\!]^2 + r_2(v, T^-)[\![T]\!] + r_3(v, \delta^-, T^-) = 0 \; , \qquad (37)$$

where

$$\left. \begin{array}{l} r_1(v) = -\dfrac{G^2 v}{2(1 - v^2)} \; , \\[4mm] r_2(v, T) = -v \left[\dfrac{(a_e)^2 - v^2}{1 - v^2} \right] \; , \\[4mm] r_3(v, \delta, T) = -\dfrac{v}{1 - v^2} \left[GT - \dfrac{1}{2} - (1 - v^2) \left(\delta - \dfrac{1}{2} + GT_T + l_T \right) \right] \; . \end{array} \right\} \qquad (38)$$

The dependence of r_2 on T is implicit in the isentropic sound speed.

3 Augmented theory

3.1 Motivation.

Although the classical thermoelastic theory of phase transitions has room for—and, in fact, requires—a kinetic relation, such a piece of constitutive information is introduced in the theory, in a sense, as a supplement. Some other theories have built-in features from which the equivalent of a kinetic relation can be *derived*. In fact, FRIED & GURTIN [14] argue that a kinetic relation is not part of the constitutive theory but follows as a consequence of new balance principles. Here, nevertheless, a viewpoint consistent with ABEYARATNE & KNOWLES [1] is taken. An augmented theory that includes viscosity, strain gradient and heat conduction is introduced. In the next section, from an admissibility criterion for a special class of solutions, namely traveling waves, a special kinetic relation in the thermomechanical case is derived. This procedure follows well established techniques used in fluid and solid mechanics (see ABEYARATNE & KNOWLES [2], HATTORI [17], ROSAKIS [22], SLEMROD [24, 25], TRUSKINOVSKY [27])

By using the classical form of the balance principles and enforcing the second law of thermodynamics for all admissible processes, GURTIN [16], generalizing a result established by COLEMAN & NOLL [10], proved that the Helmholtz potential cannot depend on higher order derivatives of the strain. In order to obtain a thermodynamically consistent theory that includes strain gradient and viscosity effects, DUNN & SERRIN [12] proposed a modification of the energy balance to take into account long range interactions by introducing the concept of *interstitial working*. An alternative approach is used by

TRUSKINOVSKY [27]. In this section, DUNN & SERRIN's model is specialized for the one-dimensional case.

3.2 Basic equations.

In the regularized theory, one introduces from the onset a new fundamental quantity called the *interstitial working p* by DUNN & SERRIN. As in the classical theory of Section 2, the momentum equation is given by (1), but by introducing the interstitial working p and considering heat conduction, the energy equation is

$$[\sigma v + p + q]_{x_1}^{x_2} = \frac{d}{dt} \int_{x_1}^{x_2} \rho \left(\epsilon + \frac{1}{2} v^2 \right) dx \ . \tag{39}$$

The Clausius-Duhem inequality (dissipation inequality) has the same form as in the classical theory with heat conduction, i.e.,

$$\Gamma(t) = \frac{d}{dt} \int_{x_1}^{x_2} \rho \eta dx - \left[\frac{q}{\theta} \right]_{x_1}^{x_2} \geq 0 \ . \tag{40}$$

At points where the field quantities have enough differentiability, the local form of the balance of linear momentum, the energy equation and the Clausius-Duhem inequality are

$$\sigma_x = \rho v_t \ , \tag{41}$$

$$(\sigma v + q + p)_x = \rho \left(\epsilon + \frac{1}{2} v^2 \right)_t \ , \tag{42}$$

$$\left(\frac{q}{\theta} \right)_x \leq \rho \eta_t \ , \tag{43}$$

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and the compatibility equation is

$$v_x = \gamma_t \ . \tag{44}$$

Using (41) in (42) provides

$$\sigma v_x + q_x + p_x = \rho \epsilon_t \ . \tag{45}$$

Furthermore, expanding the dissipation inequality (43) and using the expression of q_x provided by the energy equation (45) yields, in terms of the free energy potential ψ,

$$\rho \left(\psi_t + \theta_t \eta \right) - \sigma v_x - p_x - \frac{q \theta_x}{\theta} \leq 0 \ . \tag{46}$$

In order to introduce higher gradient effects into the theory, it is assumed that ψ, p, η, σ, q are given by functions $\hat{\psi}$, $\hat{p}$, $\hat{\eta}$, $\hat{\sigma}$, $\hat{q}$ of $\gamma, \theta, \gamma_x, \gamma_{xx}, \theta_x$ and γ_t. All functionals depend on the same set of variables since there is no *a priori* reason to discard any of them. Nevertheless, some restrictions arise in connection with the second law of thermodynamics.

3.3 Thermodynamic restrictions.

The previous constitutive assumption is compatible with thermodynamics if every admissible thermodynamic process satisfies the dissipation inequality (46). This requirement restricts the functional form of $\hat{\psi}$, $\hat{p}$, $\hat{\eta}$, $\hat{\sigma}$ and $\hat{q}$.

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Equations (46) and (44) provide

$$\rho\left[\hat{\psi}_\gamma\gamma_t + (\hat{\psi}_\theta + \hat{\eta})\theta_t + \hat{\psi}_{\gamma_x}\gamma_{xt} + \hat{\psi}_{\gamma_{xx}}\gamma_{xxt} + \hat{\psi}_{\theta_x}\theta_{xt} + \hat{\psi}_{\gamma_t}\gamma_{tt}\right] - \hat{\sigma}\gamma_t$$

$$- (\hat{p}_\gamma\gamma_x + \hat{p}_\theta\theta_x + \hat{p}_{\gamma_x}\gamma_{xx} + \hat{p}_{\gamma_{xx}}\gamma_{xxx} + \hat{p}_{\theta_x}\theta_{xx} + \hat{p}_{\gamma_t}\gamma_{xt}) - \frac{\hat{q}\theta_x}{\theta} \leq 0 .$$

This inequality has to be satisfied for all deformations and all temperatures at any point (x,t). It is possible to find a deformation and a temperature field for which, at a given point (x,t), the quantities $\theta_t, \gamma_{xt}, \gamma_{xxt}, \theta_{xt}, \gamma_{tt}, \gamma_{xxx}$ and θ_{xx} are independent of the values of $\gamma, \theta, \gamma_x, \gamma_{xx}, \theta_x$ and γ_t at the same point. Therefore, in order to satisfy the dissipation inequality, the following terms must vanish:

$$\hat{\psi}_\theta + \hat{\eta} = 0 , \quad \rho\hat{\psi}_{\gamma_x} - \hat{p}_{\gamma_t} = 0 , \tag{47}$$

$$\hat{\psi}_{\gamma_{xx}} = 0 , \quad \hat{\psi}_{\theta_x} = 0 , \quad \hat{\psi}_{\gamma_t} = 0 , \tag{48}$$

$$\hat{p}_{\gamma_{xx}} = 0 , \quad \hat{p}_{\theta_x} = 0 . \tag{49}$$

The formal role of the interstitial working and the connection between the viscosity and the strain gradient can be observed from $(47)_2$. Without the interstitial working term or without a dependence of the interstitial working on γ_t, then the Helmholtz potential would not be a function of γ_x. In view of (47)-(49), the dissipation inequality reduces to

$$\rho\hat{\psi}_\gamma\gamma_t - \hat{\sigma}\gamma_t - (\hat{p}_\gamma\gamma_x + \hat{p}_\theta\theta_x + \hat{p}_{\gamma_x}\gamma_{xx}) - \frac{\hat{q}\theta_x}{\theta} \leq 0 . \tag{50}$$

Equation (48) implies that the free energy cannot depend on these variables, hence $\psi = \hat{\psi}(\gamma, \theta, \gamma_x)$. Similarly, (49) implies that $p = \hat{p}(\gamma, \theta, \gamma_x, \gamma_t)$. Notice

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that $(47)_1$ corresponds to the same relation between entropy and free energy as in the classical theory. Since $\hat{\psi}$ does not depend on γ_t, then $(47)_2$ can be integrated, i.e.,

$$\hat{p}(\gamma, \theta, \gamma_x, \gamma_t) = \rho \hat{\psi}_{\gamma_x}(\gamma, \theta, \gamma_x)\gamma_t + p^0(\gamma, \theta, \gamma_x) \,, \tag{51}$$

where p^0 is the equilibrium part of the interstitial work. Using this expression for the interstitial working in the dissipation inequality (50) gives

$$\left\{\rho\left[\hat{\psi}_\gamma - \left(\hat{\psi}_{\gamma_x}\right)_x\right] - \hat{\sigma}\right\}\gamma_t - \left(p_\theta^0 + \frac{\hat{q}}{\theta}\right)\theta_x - (p_\gamma^0\gamma_x + p_{\gamma_x}^0\gamma_{xx}) \leq 0 \,. \tag{52}$$

The third term in this inequality is independent of θ_x and γ_t; therefore, it should satisfy $p_\gamma^0(\gamma, \theta, \gamma_x)\gamma_x + p_{\gamma_x}^0(\gamma, \theta, \gamma_x)\gamma_{xx} \geq 0$, for all $\gamma, \theta, \gamma_x, \gamma_{xx}$. Since γ_{xx} can be specified independently of γ, θ, γ_x then, necessarily, $p_{\gamma_x}^0 = 0$, but then p^0 is independent of γ_x and the same inequality implies $p_\gamma^0 = 0$. Therefore, p^0 can only be a function of θ and the dissipation inequality (52) becomes

$$\left\{\rho\left[\hat{\psi}_\gamma - \left(\hat{\psi}_{\gamma_x}\right)_x\right] - \hat{\sigma}\right\}\gamma_t - \left(p_\theta^0 + \frac{\hat{q}}{\theta}\right)\theta_x \leq 0 \,. \tag{53}$$

The equilibrium values of σ and q can be obtained by replacing θ_x and γ_t by $h\theta_x$ and $h\gamma_t$ respectively and taking the limit $h \to 0$ in the dissipation inequality (53), i.e.,

$$\left\{\rho\left[\hat{\psi}_\gamma - \left(\hat{\psi}_{\gamma_x}\right)_x\right] - \sigma_{\text{eq}}\right\}\gamma_t - \left(p_\theta^0 + \frac{q_{\text{eq}}}{\theta}\right)\theta_x \leq 0 \,, \tag{54}$$

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where $\sigma_{\text{eq}} = \hat{\sigma}(\gamma, \theta, \gamma_x, 0, 0)$ and $q_{\text{eq}} = \hat{q}(\gamma, \theta, \gamma_x, 0, 0)$. Since the first term in (54) is linear in γ_t and the second is linear in θ_x, then the equilibrium stress is given by

$$\sigma_{\text{eq}} = \rho \left[\hat{\psi}_\gamma - \left(\hat{\psi}_{\gamma_x} \right)_x \right] , \tag{55}$$

and the equilibrium heat is

$$q_{\text{eq}} = -p_\theta^0 \theta . \tag{56}$$

For *elastic* materials where $\hat{\psi}$ and $\hat{q}$ are *independent* of γ_t, the first term of the dissipation inequality (53) is linear in γ_t, hence the elastic part of the stress is completely determined by the free energy as

$$\sigma_{\text{el}} = \rho \left[\hat{\psi}_\gamma - \left(\hat{\psi}_{\gamma_x} \right)_x \right] . \tag{57}$$

Notice that the elastic stress is equal to the equilibrium stress (when $\theta_x = 0$). Define the *viscous* stress as $\sigma_{\text{v}} = \hat{\sigma} - \sigma_{\text{el}}$ and the "non-equilibrium" heat flux as $q_{\text{ne}} = \hat{q} - q_{\text{eq}}$. In the general case, the elastic stress can be obtained from the Helmholtz free energy, but for the viscous stress an *additional* constitutive assumption is required. Returning to the general case, using the expression (57) for the elastic stress and the definitions of the viscous stress and the non-equilibrium heat flux, the dissipation inequality (53) can be expressed as

$$\sigma_{\text{v}} \gamma_t + \frac{q_{\text{ne}} \theta_x}{\theta} \geq 0 .$$

Moreover, the balance of linear momentum (41) now takes the form

$$\rho \left[\hat{\psi}_\gamma - \left(\hat{\psi}_{\gamma_x} \right)_x \right]_x + (\sigma_{\mathrm{v}})_x - \rho v_t = 0 \ . \tag{58}$$

The energy equation (45), with the use of (15), (47)$_1$ and (51), yields

$$\hat{\sigma} \gamma_t + \rho \left(\hat{\psi}_{\gamma_x} \right)_x \gamma_t + p_\theta^0 \theta_x + \hat{q}_x = \rho \hat{\psi}_\gamma \gamma_t + \rho \theta \hat{\eta}_t \ .$$

From the decomposition of the stress into its elastic and viscous parts and the heat flux into its equilibrium and non-equilibrium parts, the energy equation now becomes

$$\sigma_{\mathrm{v}} \gamma_t - \left(p_\theta^0 \right)_x \theta + (q_{\mathrm{ne}})_x = \rho \theta \hat{\eta}_t \ . \tag{59}$$

This is the classical energy equation with two additional terms: the work done by the viscous stress $(\sigma_{\mathrm{v}} \gamma_t)$ and the interstitial working term $(p_\theta^0)_x \theta$. Moreover, only the non-equilibrium part of the heat flux is present.

3.4 Specific constitutive assumptions.

Introduce the following constitutive assumptions: Assume that the Helmholtz potential is of the form

$$\hat{\psi}(\gamma, \theta, \gamma_x) = \bar{\psi}(\gamma, \theta) + \frac{1}{2} \lambda \gamma_x^2 \ , \tag{60}$$

where λ is the *strain gradient coefficient*. This coefficient is formally analogous to the concept of capillarity in fluid mechanics. Moreover, assume that

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the viscous stress is given by

$$\sigma_{\mathrm{v}} = \rho \nu \gamma_t \ , \tag{61}$$

where ν is the *viscosity*, and, finally, assume that the equilibrium heat flux is zero and the non-equilibrium heat flux is only a linear function of θ_x (i.e., Fourier's law[2])

$$\hat{q}(\theta_x) = q_{\mathrm{ne}}(\theta_x) = k\theta_x \ , \tag{62}$$

where k is the *thermal conductivity*. For simplicity, the strain gradient coefficient, viscosity and thermal conductivity are assumed constant for all phases. Notice that the viscous stress is assumed as a function of γ_t only and the non-equilibrium heat flux as a function of θ_x only. These assumptions are consistent with the thermodynamical restrictions. The internal energy of the regularized theory is $\epsilon = \hat{\epsilon}(\gamma, \theta, \gamma_x) = \hat{\psi}(\gamma, \theta, \gamma_x) - \theta\hat{\psi}_\theta(\gamma, \theta, \gamma_x)$ which, by (60), can be expressed as

$$\epsilon = \hat{\epsilon}(\gamma, \theta, \gamma_x) = \bar{\epsilon}(\gamma, \theta) + \frac{1}{2}\lambda\gamma_x^2 \ , \tag{63}$$

where $\bar{\epsilon}(\gamma, \theta) = \bar{\psi}(\gamma, \theta) - \theta\bar{\psi}_\theta(\gamma, \theta)$. Moreover, since the equilibrium heat flux is zero, then, from (56), it follows that the equilibrium part of the interstitial work, p^0, can at most be a constant. Since the energy equation and the dissipation inequality only involve derivatives of p^0 then, without loss of

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[2]Recall that in the linear theory (linearized about a reference temperature), the heat flux can only depend linearly on the temperature gradient (see, e.g., CARLSON [7]).

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generality for a material that follows Fourier's law, one can take $p^0 = 0$.
With assumptions (60)-(62) enforced, the stress becomes

$$\hat{\sigma}(\gamma, \theta, \gamma_{xx}, \gamma_t) = \rho \left[\bar{\psi}_\gamma(\gamma, \theta) - \lambda \gamma_{xx} + \nu \gamma_t \right] , \qquad (64)$$

the balance of linear momentum (58) takes the form

$$\left(\bar{\psi}_\gamma \right)_x - \lambda \gamma_{xxx} + \nu \gamma_{xt} - v_t = 0 , \qquad (65)$$

and the energy equation (59) reduces to

$$\nu \gamma_t^2 + \frac{k}{\rho} \theta_{xx} + \theta \left(\bar{\psi}_\theta \right)_t = 0 . \qquad (66)$$

Recall that the strain and particle velocity are related through (44). The dissipation inequality (53) can be expressed as

$$\rho \nu \gamma_t^2 + \frac{k}{\theta} \theta_x^2 \geq 0 , \qquad (67)$$

which is satisfied if $\nu \geq 0$ and $k \geq 0$. By setting $\nu = \lambda = 0$ in equations (65) and (66), one recovers the corresponding equations for a classical thermoelastic material with heat conduction.

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4 Structured wave: Viscosity, strain gradient and heat conduction

4.1 Generalities.

The traveling wave problem is analyzed here within the context of the augmented theory. There are several possibilities for connecting the augmented theory of Section 3 to the sharp interface theory of Section 2. The three structuring mechanisms are related to viscous, strain gradient and heat conduction effects. The case when the viscosity and strain gradient coefficient are assumed small (in a sense to be specified) is analyzed and it is shown that a kinetic relation can be inherited when $\lambda, \nu, k \to 0$ and that the augmented theory reduces to the sharp interface theory. As a motivation for the use of viscous and strain gradient effects, it was shown in [28] that when the only structuring mechanism is heat conductivity, only *supersonic* traveling waves can be achieved and no kinetic relation can be derived. It is also important to remark that the presence of heat conduction induces some structure to the phase boundary but, more significantly, it permits specification of different temperatures at $+\infty$ and $-\infty$. This in turn allows an appropriate connection with the *adiabatic* limit case.

After introducing some general features of a structured traveling wave in Section 4.2, the basic equations are developed in Section 4.3. Classical techniques of singular perturbation theory[3] are then used to identify the region where the viscosity and strain gradient play an important role (i.e.,

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[3]See, e.g., KEVORKIAN & COLE [18], WHITHAM [29].

the "inner" solution) and the region where heat conduction is the relevant structuring mechanism (i.e., the "outer" solution). A uniformly valid approximation is then obtained from the asymptotic matching of the inner and outer solutions and a kinetic relation of the form (29) is derived for a *subsonic* traveling phase boundary.

4.2 Traveling wave: Preliminaries.

A steady, structured traveling wave corresponds to the case when all fields satisfy (41)-(44) and depend only on the variable $\xi = x - \dot{s}t$, where $\dot{s}$, the wave speed, is a constant. A moving discontinuity can be viewed, within the context of the adiabatic, sharp interface theory, as the limit of a structured wave within the framework of the augmented theory. Hence, in an infinitely long bar, the conditions at $\pm\infty$ for a structured wave in the augmented theory should correspond to the front and back states of a moving discontinuity in the theory without augmentation. The precise statement of the traveling wave problem will be given in Section 4.4. In this section, some general characteristics of the traveling wave are recorded for future use. Notice that although in the classical theory of Section 2 the function $\bar{\psi}$ corresponds to the Helmholtz free energy, in the augmented theory, the free energy is given by $\hat{\psi}$. Assume there exists a structured, steady traveling wave for $\xi \in \mathbb{R}$.

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From (41), (42) and (44) it follows that

$$\sigma' + \rho\dot{s}v' = 0 \ , \tag{68}$$

$$v' + \dot{s}\gamma' = 0 \ , \tag{69}$$

$$(\sigma v)' + q' + p' + \rho\dot{s}\left(\epsilon + \frac{1}{2}v^2\right)' = 0 \ , \tag{70}$$

where $(\cdot)'$ denotes differentiation with respect to ξ. Integration of these equations yields

$$\sigma + \rho\dot{s}v = H_1 \ , \tag{71}$$

$$v + \dot{s}\gamma = H_2 \ , \tag{72}$$

$$\sigma v + q + p + \rho\dot{s}\left(\epsilon + \frac{1}{2}v^2\right) = H_3 \ , \tag{73}$$

where the H_i are integration constants. Let the conditions at $\xi \to \pm\infty$ be given by

$$\gamma(-\infty) = \gamma^- \ , \quad \gamma(+\infty) = \gamma^+ \ , \tag{74}$$

$$v(-\infty) = v^- \ , \quad v(+\infty) = v^+ \ , \tag{75}$$

$$\theta(-\infty) = \theta^- \ , \quad \theta(+\infty) = \theta^+ \ , \tag{76}$$

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and all derivatives of these quantities vanish when $\xi \to \pm\infty$. Hence, the integration constants must satisfy

$$H_1 = \sigma^+ + \rho\dot{s}v^+ = \sigma^- + \rho\dot{s}v^- , \tag{77}$$

$$H_2 = v^+ + \dot{s}\gamma^+ = v^- + \dot{s}\gamma^- , \tag{78}$$

$$H_3 = \sigma^+ v^+ + \rho\dot{s}\left(\epsilon^+ + \frac{1}{2}(v^+)^2\right) = \sigma^- v^- + \rho\dot{s}\left(\epsilon^- + \frac{1}{2}(v^-)^2\right) , \tag{79}$$

where $\sigma^{\pm} = \hat{\sigma}(\gamma^{\pm}, \theta^{\pm}, 0, 0)$ and $\epsilon^{\pm} = \hat{\psi}(\gamma^{\pm}, \theta^{\pm}, 0) - \theta^{\pm}\hat{\psi}_\theta(\gamma^{\pm}, \theta^{\pm}, 0)$. With the foregoing constitutive assumptions (60)-(62), the stress $\sigma^{\pm}$, given by (64), is $\sigma^{\pm} = \rho\bar{\psi}_\gamma(\gamma^{\pm}, \theta^{\pm})$ and the internal energy $\epsilon^{\pm}$ becomes $\epsilon^{\pm} = \bar{\psi}(\gamma^{\pm}, \theta^{\pm}) - \theta^{\pm}\bar{\psi}_\theta(\gamma^{\pm}, \theta^{\pm})$. Therefore, from (77)-(79), the values given in (74)-(76) must satisfy the adiabatic jump conditions (9)-(11).If a traveling wave solution exists then, from (59), it necessarily satisfies

$$-\rho\dot{s}\eta' = \rho\dot{s}^2\nu\frac{\gamma'^2}{\theta} + k\frac{\theta''}{\theta} .$$

Integrate from $\xi \to -\infty$ to $\xi \to \infty$ to get

$$-\rho\dot{s}[\![\eta]\!] = \int_{-\infty}^{\infty}\left\{\rho\dot{s}^2\nu\frac{\gamma'^2}{\theta} + k\frac{\theta''}{\theta}\right\}d\xi ,$$

where $[\![\eta]\!] = \eta^+ - \eta^- = -\bar{\psi}_\theta(\gamma^+, \theta^+) + \bar{\psi}_\theta(\gamma^-, \theta^-)$. Integrating by parts the second term in the integral and using the conditions at $\pm\infty$ provides

$$-\rho\dot{s}[\![\eta]\!] = \int_{-\infty}^{\infty}\left\{\rho\dot{s}^2\nu\frac{\gamma'^2}{\theta} + k\left(\frac{\theta'}{\theta}\right)^2\right\}d\xi \geq 0 .$$

To make the connection with the classical adiabatic theory, consider the driving traction f given by (26). Thus, the values in (74)-(76) must also satisfy $f\dot{s} \geq 0$, which corresponds to the entropy jump inequality (28). The previous analysis shows that the field values at $\xi \to \pm\infty$ for the traveling wave problem must satisfy all the corresponding jump conditions of the classical adiabatic problem. Moreover, the condition for the existence of a traveling wave solution for the augmented theory should provide an additional relation for the phase boundary velocity $\dot{s}$ in terms of the driving traction f.

4.3 Basic equations.

Evaluate the constants H_i in (71)-(73) using the conditions at an *arbitrary* point $\xi = \xi_0$. These equations can be written as follows:

$$\sigma - \sigma_0 + \rho\dot{s}(v - v_0) = 0 \ , \tag{80}$$

$$(v - v_0) + \dot{s}(\gamma - \gamma_0) = 0 \ , \tag{81}$$

$$(\sigma v - \sigma_0 v_0) + q - q_0 + p - p_0 + \rho\dot{s}\left(\epsilon - \epsilon_0 + \frac{1}{2}(v^2 - v_0{}^2)\right) = 0 \ , \tag{82}$$

where $\sigma_0 = \hat{\sigma}(\gamma_0, \theta_0, \gamma_0'', -\dot{s}\gamma_0')$, etc., and $\gamma_0 = \gamma(\xi_0)$, etc. The velocity v can be eliminated from (80) and (82) by use of (81). The momentum equation (80) becomes

$$\sigma - \rho\dot{s}^2\gamma = \sigma_0 - \rho\dot{s}^2\gamma_0 \ , \tag{83}$$

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and the energy equation (82) can be expressed as

$$q - q_0 + p - p_0 = -\dot{s} \left[\rho(\epsilon - \epsilon_0) - \left(\frac{\sigma + \sigma_0}{2} \right) (\gamma - \gamma_0) \right] . \qquad (84)$$

Alternatively, using the expression for σ given by (83), the previous equation can be written as

$$q - q_0 + p - p_0 + \rho\dot{s} \left[(\epsilon - \epsilon_0) - \frac{\dot{s}^2}{2} (\gamma - \gamma_0)^2 - \frac{\sigma_0}{\rho}(\gamma - \gamma_0) \right] = 0 . \qquad (85)$$

Equation (85) is therefore a combination of the compatibility, momentum and energy equations. Moreover, it is clear that by choosing the conditions *behind* (resp. *ahead*) a right-traveling wave in (77)-(79), i.e., the "−" side (resp. the "+" side), (83) and (85) are also valid with the subscript 0 replaced by "−" (resp. by "+") and with $q^- = p^- = 0$ (resp. $q^+ = p^+ = 0$). Using the constitutive assumptions (60)-(62), the heat flux q and the interstitial work p are, for a traveling wave, given by

$$q = k\theta' , \quad p = -\rho\dot{s}\lambda\gamma'^2 . \qquad (86)$$

From (64) and (63), the stress and the internal energy are given by

$$\sigma = \rho \left[\bar{\psi}_\gamma(\gamma, \theta) - \lambda\gamma'' - \nu\dot{s}\gamma' \right] \qquad (87)$$

$$\epsilon = \bar{\epsilon}(\gamma, \theta) + \frac{1}{2}\lambda\gamma'^2 . \qquad (88)$$

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Using (86)-(88) in the governing equations (83) and (85) gives

$$\lambda(\gamma'' - \gamma_0'') + \nu\dot{s}(\gamma' - \gamma_0') - [\bar{\psi}_\gamma(\gamma, \theta) - \bar{\psi}_\gamma(\gamma_0, \theta_0)] + \dot{s}^2(\gamma - \gamma_0) = 0 \ , \tag{89}$$

$$\frac{k}{\rho}(\theta' - \theta_0') + \dot{s}\left\{\bar{\epsilon}(\gamma, \theta) - \bar{\epsilon}(\gamma_0, \theta_0) - \frac{1}{2}\lambda\left(\gamma'^2 - \gamma_0'^2\right)\right.$$
$$\left. - \frac{1}{2}\dot{s}^2\left(\gamma - \gamma_0\right)^2 - [\bar{\psi}_\gamma(\gamma_0, \theta_0) - \lambda\gamma_0'' - \nu\dot{s}\gamma_0'](\gamma - \gamma_0)\right\} = 0 \ . \tag{90}$$

Introduce a new function $w = \gamma'$. Equations (89) and (90) can be expressed as a system of first order ordinary differential equations:

$$\begin{cases} \gamma' = w, \\\\ w' - w_0' = -\dfrac{1}{\lambda}\left\{\nu\dot{s}(w - w_0) - [\bar{\psi}_\gamma(\gamma, \theta) - \bar{\psi}_\gamma(\gamma_0, \theta_0)] + \dot{s}^2(\gamma - \gamma_0)\right\}, \\\\ \theta' - \theta_0' = -\dfrac{\rho\dot{s}}{k}\left\{\bar{\epsilon}(\gamma, \theta) - \bar{\epsilon}(\gamma_0, \theta_0) - \dfrac{\lambda}{2}(w^2 - w_0^2) - \dfrac{\dot{s}^2}{2}(\gamma - \gamma_0)^2 \right. \\\\ \left. \qquad\qquad - [\bar{\psi}_\gamma(\gamma_0, \theta_0) - \lambda w_0' - \nu\dot{s}w_0](\gamma - \gamma_0)\right\}. \end{cases} \tag{91}$$

The following stability analysis, with some modifications, follows from NGAN & TRUSKINOVSKY [20]. Let $(\gamma_*, w_*, \theta_*)$ be an equilibrium point of this dynamical system. Therefore, from (91) and assuming $\dot{s} \neq 0$, these points satisfy the jump conditions of the classical adiabatic theory for a given state (γ^+, θ^+); see relations (13) and (14). The states at $\xi \to \pm\infty$ given by (74)-(76) are equilibrium points. To analyze the nature of the equilibria, consider

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the linearized system around an equilibrium point, i.e., $W' = AW$, where $W = (\gamma, w, \theta)$ and

$$
A = \begin{bmatrix}
0 & 1 & 0 \\[2ex]
-\dfrac{1}{\lambda}\left[\dot{s}^2 - \psi_{\gamma\gamma}^*\right] & -\dfrac{\nu\dot{s}}{\lambda} & \dfrac{\psi_{\gamma\theta}^*}{\lambda} \\[2ex]
\dfrac{\rho\dot{s}}{k}\theta_*\psi_{\gamma\theta}^* & 0 & \dfrac{\rho\dot{s}}{k}\theta_*\psi_{\theta\theta}^*
\end{bmatrix} , \tag{92}
$$

where $\psi_{\gamma\gamma}^* = \bar{\psi}_{\gamma\gamma}(\gamma_*, \theta_*)$, $\psi_{\gamma\theta}^* = \bar{\psi}_{\gamma\theta}(\gamma_*, \theta_*)$, $\psi_{\theta\theta}^* = \bar{\psi}_{\theta\theta}(\gamma_*, \theta_*)$. Notice that to obtain the term A_{31}, the relation $\bar{\epsilon}_\gamma = \bar{\psi}_\gamma - \theta\bar{\psi}_{\gamma\theta}$ was used. The term A_{33} was obtained using $\bar{\epsilon}_\theta = -\theta\bar{\psi}_{\theta\theta}$. Let $\beta = \beta_i$, $i = 1, 2, 3$, be the eigenvalues of A. The characteristic polynomial of A is $\beta^3 - I_1\beta^2 + I_2\beta - I_3 = 0$, where I_i, $i = 1, 2, 3$, are the principal invariants of A. A direct calculation gives, using the material parameters introduced in Section 2.2, gives

$$
I_1 = -\dot{s}\left(\frac{\nu}{\lambda} + \frac{\rho c_*}{k_*}\right) , \tag{93}
$$

$$
I_2 = -\frac{1}{\lambda}\left[a_*^2 - \dot{s}^2\left(\frac{\rho c_*\nu}{k_*} + 1\right)\right] , \tag{94}
$$

$$
I_3 = \frac{\rho c_*\dot{s}}{\lambda k_*}\left[a_{e*}^2 - \dot{s}^2\right] . \tag{95}
$$

Define

$$
\iota_1 = I_3 + \frac{I_1 I_2}{3} - \frac{2}{27}I_1^3 , \quad \iota_2 = \frac{I_2}{3} - \frac{I_1^2}{9} , \quad \iota_3 = \iota_1^2 + 4\iota_2^3 , \tag{96}
$$

then, when $\iota_3 < 0$, all three eigenvalues are real and different; when $\iota_3 = 0$, all

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eigenvalues are real and two of them are equal and when $\iota_3 > 0$ one solution is real and the two other are complex. The eigenvalues β_i satisfy $\beta_1 + \beta_2 + \beta_3 = I_1$ and $\beta_1\beta_2\beta_3 = I_3$, hence if the three eigenvalues are real, and since $I_1 < 0$ when $\dot{s} > 0$, then the three eigenvalues cannot be all positive. Therefore, if $I_3 > 0$, the equilibrium saddle point has a two-dimensional *stable* manifold and a one-dimensional *unstable* manifold. If $\dot{s} < 0$, then the equilibrium point has a two-dimensional *unstable* manifold and a one-dimensional *stable* manifold. If $I_3 < 0$ then the situation is reversed.

4.4   Traveling phase boundary.

Since the fields under consideration are piecewise differentiable, the traveling phase boundary problem has to be divided into three sub-problems. Suppose that the conditions at $\xi \rightarrow +\infty$ correspond to the *low strain* phase and the conditions at $\xi \rightarrow -\infty$ correspond to the *high strain* phase. Presumably there is an interval, say $(0, b)$, where the points are in the unstable phase. From the above considerations and in view of the smoothness requirements of the traveling wave, the solution must satisfy conditions (74), (76) and the strain, strain gradient and temperature must be *continuous* at $\xi = 0$ and $\xi = b$. In particular, $\gamma(0^\pm) = \gamma_m(\theta_0)$ and $\gamma(b^\pm) = \gamma_M(\theta_b)$, where the functions γ_m and γ_M are given by (30) and the temperatures $\theta_0 = \theta(0^\pm)$ and $\theta_b = \theta(b^\pm)$ are unknown. Additionally, for the class of traveling waves considered here, the *phase segregation* conditions must be enforced, i.e., the solution must be such that the material is in its high strain phase in $(-\infty, 0)$, unstable phase in $(0, b)$ and low strain phase in $(b, +\infty)$. Moreover, the temperature has to

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be below the critical value θ_C. These conditions can be expressed as

$$\left.\begin{array}{ll} -1 < \gamma(\xi) \leq \gamma_M(\theta(\xi)) & \text{for } -\infty < \xi < 0 , \\[2mm] \gamma_M(\theta(\xi)) \leq \gamma(\xi) \leq \gamma_m(\theta(\xi)) & \text{for } 0 < \xi < b , \\[2mm] \gamma(\xi) \geq \gamma_m(\theta(\xi)) & \text{for } b < \xi < +\infty , \\[2mm] \theta(\xi) \leq \theta_C & \text{for } -\infty < \xi < +\infty . \end{array}\right\} \quad (97)$$

Structured phase boundary traveling wave problem: *Given one end state, say (γ^-, θ^-) at $\xi \to -\infty$, (or, alternatively, (γ^+, θ^+) at $\xi \to +\infty$) find all admissible states (γ^+, θ^+) at $\xi \to +\infty$ in the high strain phase such that (γ^-, θ^-) and (γ^+, θ^+) can be connected via a traveling wave. A connection between the end states is achieved if there exist functions $\gamma(\xi)$ and $\theta(\xi)$, $\xi \in \mathbb{R}$, that satisfy the phase segregation conditions (97) and the following three problems:*

Problem 1: *Low strain phase.* Suppose that for $\xi \in (-\infty, 0)$ the material is in its low strain phase. Using the conditions at $-\infty$ in system (91) and the corresponding expressions of $\bar{\psi}(\gamma, \theta)$, $\bar{\epsilon}(\gamma, \theta)$, ϵ^- and σ^- given by equations

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(15)-(17) and (34), the governing equations are

$$
\begin{cases}
\gamma' = w, \\[2ex]
w' = -\dfrac{1}{\lambda}\left\{\nu\dot{s}w - (a^2 - \dot{s}^2)(\gamma - \gamma^-) + \alpha a^2(\theta - \theta^-)\right\}, \\[2ex]
\theta' = -\dfrac{\rho\dot{s}}{k}\left\{\dfrac{1}{2}\left(a^2 - \dot{s}^2\right)(\gamma - \gamma^-)^2 + \alpha a^2\theta^-(\gamma - \gamma^-)\right. \\[2ex]
\qquad\qquad \left. + c(\theta - \theta^-) - \dfrac{\lambda}{2}w^2\right\},
\end{cases}
\tag{98}
$$

subject to the following boundary conditions:

$$
\gamma(-\infty) = \gamma^- , \quad \theta(-\infty) = \theta^- , \quad \gamma'(-\infty) = 0 , \tag{99}
$$

$$
\gamma(0^-) = \gamma_0 = \gamma_C + M(\theta_0 - \theta_C) , \quad [\theta_0 \equiv \theta(0^-)]. \tag{100}
$$

The temperature θ_0 is not known *a priori.*

Problem 2: *Unstable phase.* Suppose that for $\xi \in (0, b)$ the material is in its unstable phase. The governing equations are

$$
\begin{cases}
\gamma' = w, \\
\\
w' = -\dfrac{1}{\lambda}\Bigg\{ \nu \dot{s} w - (a^2 - \dot{s}^2)(\gamma - \gamma^-) + \alpha a^2(\theta - \theta^-) \\
\qquad\quad +a^2 \dfrac{\gamma_T(\gamma - \gamma_M(\theta))}{\gamma_m(\theta) - \gamma_M(\theta)} \Bigg\}, \\
\\
\theta' = -\dfrac{\rho \dot{s}}{k}\Bigg\{ \dfrac{1}{2}\left(a^2 - \dot{s}^2\right)(\gamma - \gamma^-)^2 + \alpha a^2 \theta^-(\gamma - \gamma^-) + c(\theta - \theta^-) - \dfrac{\lambda}{2}w^2 \\
\qquad\quad + \dfrac{a^2 \gamma_T}{2(M - m)}\left[\dfrac{(2\theta - \theta_C)(\gamma - \gamma_C)^2}{(\theta - \theta_C)^2} - M^2 \theta_C - 2M(\gamma - \gamma_C)\right] \Bigg\},
\end{cases}
\tag{101}
$$

subject to the following initial conditions:

$$
\gamma(0^+) = \gamma_0 = \gamma_C + M(\theta_0 - \theta_C), \quad \theta(0^+) = \theta_0, \tag{102}
$$

$$
\gamma'(0^+) = \gamma'(0^-). \tag{103}
$$

Problem 3: *High strain phase.* Suppose that for $\xi \in (b, +\infty)$ the material is in its high strain phase. The governing equations are

$$
\begin{cases}
\gamma' = w, \\[2ex]
w' = -\dfrac{1}{\lambda}\left\{ \nu \dot{s} w - (a^2 - \dot{s}^2)(\gamma - \gamma^+) + \alpha a^2(\theta - \theta^+) \right\}, \\[3ex]
\theta' = -\dfrac{\rho \dot{s}}{k}\left\{ \dfrac{1}{2}\left(a^2 - \dot{s}^2\right)(\gamma - \gamma^+)^2 + \alpha a^2 \theta^+ (\gamma - \gamma^+) \right. \\[2ex]
\qquad\qquad \left. +\, c(\theta - \theta^+) - \dfrac{\lambda}{2} w^2 \right\},
\end{cases}
\tag{104}
$$

subject to the following boundary conditions:

$$
\gamma(b^+) = \gamma_b = \gamma_C + m(\theta_b - \theta_C)\,, \quad [\theta_b \equiv \theta(b^+)], \tag{105}
$$

$$
\gamma(+\infty) = \gamma^+\,, \quad \theta(+\infty) = \theta^+\,, \quad \gamma'(+\infty) = 0\,, \tag{106}
$$

$$
\gamma'(b^+) = \gamma'(b^-) = \gamma'_b\,. \tag{107}
$$

The temperature θ_b, the strain gradient γ'_b and the width of the unstable phase b are unknown *a priori*.

4.5 Nondimensional parameters.

It is convenient to introduce a length parameter based on the viscosity and strain gradient coefficient and to use it to obtain nondimensional equations. Recall that the viscosity is given in terms of $L^2 T^{-1}$, where L is length and

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T is time, and the strain gradient coefficient in terms of $L^4 T^{-2}$. Let

$$z = \frac{\rho c a}{k} \xi \,, \quad \omega = \frac{\nu}{\sqrt{\lambda}} \,, \quad \varpi = \frac{k}{\rho c \sqrt{\lambda}} \,.$$

Therefore, the system (98) can be expressed as

$$\begin{cases} \delta' = w, \\[2em] w' = -\omega \varpi v w + \varpi^2 \left[(1 - v^2)(\delta - \delta^-) - G(T - T^-) \right], \\[2em] T' = -v \left\{ \frac{1}{2} \left(1 - v^2 \right) \left(\delta - \delta^- \right)^2 + G T^- (\delta - \delta^-) + (T - T^-) - \frac{1}{2\varpi^2} w^2 \right\}, \end{cases} \tag{108}$$

where $(\cdot)' \equiv d/dz$. The boundary condition at $z = 0$ is

$$\delta(0) = \delta_C + M(T(0) - T_C) \,. \tag{109}$$

The nondimensional expression for the unstable phase will be given in section 4.6. The system (104) can be written as

$$\begin{cases} \delta' = w, \\[2em] w' = -\omega \varpi v w + \varpi^2 \left[(1 - v^2)(\delta - \delta^+) - G(T - T^+) \right], \\[2em] T' = -v \left\{ \frac{1}{2} \left(1 - v^2 \right) \left(\delta - \delta^+ \right)^2 + G T^+ (\delta - \delta^+) + (T - T^+) - \frac{1}{2\varpi^2} w^2 \right\}, \end{cases} \tag{110}$$

and the boundary condition (105) at $z = b$ is

$$\delta(b) = \delta_C + m(T(b) - T_C) .\qquad(111)$$

The boundary condition (107) will be analyzed in Section 4.7. The dimensionless driving traction is defined as

$$f = -[\![s]\!]\langle T \rangle = \frac{f}{\rho a^2 \gamma_T^2} \; ;$$

hence, if the conditions at $+\infty$ correspond to the high strain phase, then, from (35),

$$f = -\left[G\left([\![\delta]\!] - 1 \right) + \log \frac{T^+}{T^-} - \frac{l_T}{T_T} \right] \langle T \rangle .\qquad(112)$$

From $(108)_2$, the temperature can be written in terms of the strain and its derivatives as

$$T(z) - T^- = \frac{1}{G}\left[(1 - v^2)(\delta(z) - \delta^-) - \frac{1}{\varpi}\omega v\delta'(z) - \frac{1}{\varpi^2}\delta''(z) \right] ,$$
$$\qquad(113)$$

hence, equation $(108)_3$ can be expressed as a single equation for the strain, i.e.,

$$\delta''' - l_1\delta'' + l_2\delta' - l_3(\delta - \delta^-) + \frac{Gv}{2}\left[(\delta')^2 - \varpi^2(1 - v^2)\left(\delta - \delta^-\right)^2 \right] = 0 .$$
$$\qquad(114)$$

A similar equation can be obtained for the high strain phase.

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4.6 Perturbation analysis.

To obtain an approximation of the solution in the metastable phases, consider a singular perturbation of the equations. Let

$$\varepsilon = \frac{1}{\varpi} \, ,$$

and consider the case where $\lambda \ll 1$, $\nu \ll 1$ but the ratio ω remains *fixed*. Hence, assume that ε is a small parameter. For definiteness, the analysis is carried out for the low strain phase (it is formally the same for the high strain phase). As a general scheme of notation in this section, an overbar represents a quantity related to the inner expansion whereas a quantity without an overbar usually represents a value related to the outer expansion. A prime denotes differentiation with respect to the outer coordinate and a dot denotes differentiation with respect to the inner coordinate.

Outer solution

Assume that the asymptotic expansion for δ corresponds to a power series in ε for fixed $z \neq 0$, i.e.,

$$\delta(z) - \delta^- \sim \phi_0(z) + \varepsilon\phi_1(z) + \dots \quad \text{as } \varepsilon \to 0 \, .$$

This corresponds to the outer solution. Using this representation for δ in equation (114), collecting terms in powers of ε and setting each of the coefficients equal to zero gives, for the first term,

$$\phi_0' = r_2\phi_0 + r_0\phi_0^2 \, ,$$

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where r_2 is defined by (38) and

$$r_0(v) = -\frac{Gv}{2} \, . \tag{115}$$

There are two functions that satisfy the equation for ϕ_0 (one of them being the trivial solution). For the nontrivial solution the first term of the expansion is given by

$$\phi_0(z) = \frac{r_2}{r_0} \left\{ \frac{r_2}{r_0} c_0 \exp[-r_2 z] - 1 \right\}^{-1} , \tag{116}$$

where c_0 is a constant. In order to enforce the condition that $\phi_0(z) \to 0$ as $z \to -\infty$, it is required that $r_2 = r_2(v, T^-) > 0$ in the low strain phase, but no further restriction is placed upon c_0. For the high strain phase the restriction is that $r_2 = r_2(v, T^+) < 0$. Observe that $\forall n \in \mathbb{N}$, $\phi_0^{(n)}(z) \to 0$ as $z \to -\infty$. The same occurs for $z \to +\infty$. Formally, the strain gradient is given by $\delta'(z) \sim \phi_0'(z) + \dots$, and the temperature is given, from (113), by

$$T(z) - T^- \sim \frac{1 - v^2}{G} \phi_0(z) + \dots ; \tag{117}$$

therefore, the boundary condition $T(z) - T^- \to 0$ as $z \to -\infty$ is satisfied.

Inner solution.

For the inner solution (close to $z = 0$), consider a new coordinate defined as

$$x \equiv \frac{z}{\varepsilon} = \varpi z \, .$$

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Assume the following asymptotic expansion for fixed x:

$$\delta(x) - \delta^- \sim \bar{\phi}_0(x) + \varepsilon \bar{\phi}_1(x) + \dots .$$

Proceeding as in the previous section, the equation to determine the first term of the expansion is, from (114),

$$\dddot{\bar{\phi}}_0 + v\omega \ddot{\bar{\phi}}_0 - (1 - v^2)\dot{\bar{\phi}}_0 = 0 .$$

The solution $\bar{\phi}_0$ is given by the sum of two exponentials plus a constant. The exponents are $\overset{\pm}{\beta}x$, where

$$\overset{\pm}{\beta} = \frac{1}{2}(-v\omega \pm \sqrt{v^2\omega^2 + 4(1 - v^2)}) . \tag{118}$$

The exponents can be either real or complex. For the subsonic range (subsonic with respect to the isothermal sound speed), the exponents are real: $\overset{+}{\beta} > 0$, $\overset{-}{\beta} < 0$ for $0 < v < 1$ and $\overset{\pm}{\beta} > 0$ for $-1 < v < 0$. In the low strain phase (where $x < 0$), since the inner and outer solution must match in some region (as explained below), the exponential(s) with negative exponent(s)—which would provide an unbounded term in the limit—should be discarded. For the high strain phase, the solution with positive exponent(s) should be abandoned. If both exponents have the appropriate sign, then, in general,

$$\bar{\phi}_0(x) = \bar{c}_0 e^{\overset{+}{\beta}x} + \bar{c}_1 e^{\overset{-}{\beta}x} + \bar{c}_2 . \tag{119}$$

Notice that, from (96) in nondimensional form, the eigenvalues of the system linearized about the equilibrium point for the metastable phases are real and

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different if

$$-\frac{1}{27}(1 - v^2)^2 \left[v^2 \omega^2 + 4(1 - v^2) \right] + O(\varepsilon) < 0 \ ,$$

i.e., if $v^2 \omega^2 + 4(1 - v^2) > 0$ for small ε. Therefore, for small ε, the equilibrium points of the systems (108) (low strain phase) and (110) (high strain phase) have a two-dimensional stable manifold and a one-dimensional unstable manifold for $0 < v < 1$ and a one-dimensional stable manifold and a two-dimensional unstable manifold for $-1 < v < 0$.

Unstable phase.

For the *unstable* phase, the system of equations (101) in nondimensional form and expressed in *inner* coordinates becomes

$$\begin{cases} \dot{\delta} = \bar{w}, \\[2ex] \dot{\bar{w}} = -\omega v \bar{w} + \left[(1 - v^2)(\delta - \delta^-) - G(T - T^-) + \dfrac{\delta - \delta_C - M(T - T_C)}{(M - m)(T - T_C)} \right], \\[3ex] \dot{T} = -\dfrac{v}{\varpi} \left\{ \dfrac{1}{2} \left(1 - v^2 \right) \left(\delta - \delta^- \right)^2 + G T^- (\delta - \delta^-) + (T - T^-) - \bar{w}^2 \right. \\[2ex] \qquad \left. + \dfrac{1}{2(M - m)} \left[\dfrac{(2T - T_C)(\delta - \delta_C)^2}{(T - T_C)^2} - M^2 T_C - 2M(\delta - \delta_C) \right] \right\}. \end{cases} \tag{120}$$

Assuming that the strain, strain gradient and the temperature are bounded throughout the unstable phase, it is possible to conclude from $(120)_3$ that

$$T(\mathsf{x}) - T_0 = O(\varepsilon) \ ,$$

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where T_0 is the (unknown) value of the temperature at $x = 0$. Therefore, assuming that

$$\delta(x) - \delta^- \sim \bar{\phi}_0(x) + \varepsilon\bar{\phi}_1(x) + \dots \, ,$$

equations $(120)_{1,2}$ give, for the first term,

$$\ddot{\bar{\phi}}_0(x) + \omega v \dot{\bar{\phi}}_0(x) + k_1\bar{\phi}_0(x) + k_2 = 0 \, ,$$

where

$$\left.\begin{aligned}
k_1 &= -\left[(1 - v^2) + \frac{1}{(M - m)(T_0 - T_C)}\right] \, , \\
k_2 &= G(T_0 - T^-) - \frac{\delta^- - \delta_C - M(T_0 - T_C)}{(M - m)(T_0 - T_C)} \, .
\end{aligned}\right\} \qquad (121)$$

Hence,

$$\bar{\phi}_0(x) = \bar{c}_1^u e^{\overset{+}{\beta}_u x} + \bar{c}_2^u e^{\overset{-}{\beta}_u x} - \frac{k_2}{k_1} \, , \qquad (122)$$

where

$$\overset{\pm}{\beta}_u = \frac{1}{2}\left(-v\omega \pm \sqrt{v^2\omega^2 - 4k_1}\right) \, . \qquad (123)$$

Notice that the exponents can be either real or complex. The following quantities will be useful in the foregoing analysis:

$$\left.\begin{aligned}
P(v) &= \overset{+}{\beta} - \overset{-}{\beta} = \sqrt{v^2\omega^2 + 4(1 - v^2)} \, , \\
Q(v, T_0) &= \overset{+}{\beta}_u - \overset{-}{\beta}_u = \sqrt{v^2\omega^2 - 4k_1} \, .
\end{aligned}\right\} \qquad (124)$$

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4.7 Subsonic case.

To obtain a uniformly valid approximation of the solution in the metastable phases, the inner and outer solutions must match. For the subsonic case (subsonic with respect to the isothermal sound speed) the regions where the different approximations are valid are shown in Figure 2.

Low strain phase.

Suppose that $0 < v < 1$. From $(38)_2$ it follows that $r_2(v, T^{\pm}) < 0$, hence the nontrivial outer solution for the low strain phase has to be abandoned in favor of the trivial solution. Furthermore, since $\overset{+}{\beta} > 0$ and $\overset{-}{\beta} < 0$, the inner solution for the low strain phase involves, up to $O(\varepsilon)$, only the exponential with exponent $\overset{+}{\beta}x$. From (119), the inner solution is given by

$$\delta(x) - \delta^- = \bar{\phi}_0(x) + O(\varepsilon) , \qquad (125)$$

where $\bar{\phi}_0(x) = \bar{c}_0 e^{\overset{+}{\beta}x} + \bar{c}_2$. Before enforcing the boundary condition at $x = 0$, it is convenient first to analyze the restrictions imposed by the asymptotic matching of the inner and outer solutions. The inner expansion, rewritten in outer variables (i.e., z) and expanded for small ε and fixed z is given by $\bar{c}_2 + \ldots$. The one-term outer expansion of the one-term inner expansion rewritten in inner coordinates is, clearly, $\bar{c}_2$. For this expansion to match the (trivial) outer expansion, it is required that

$$\bar{c}_2 = 0 . \qquad (126)$$

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The temperature can be expressed, from (113) in inner coordinates, as

$$T(\mathsf{x}) - T^- = \frac{1}{\mathsf{G}} \left[(1 - \mathsf{v}^2)(\delta(\mathsf{x}) - \delta^-) - \omega \mathsf{v} \dot{\delta}(\mathsf{x}) - \ddot{\delta}(\mathsf{x}) \right] . \qquad (127)$$

The strain and the temperature at $\mathsf{x} = 0$ are related through the boundary condition (109). From (125)-(127), the first term of the temperature's expansion at $\mathsf{x} = 0$ is

$$\frac{1}{\mathsf{G}} \left[(1 - \mathsf{v}^2)\bar{\phi}_0(0) - \omega \mathsf{v} \dot{\bar{\phi}}_0(0) - \ddot{\bar{\phi}}_0(0) \right] = \frac{1}{\mathsf{G}}(1 - \mathsf{v}^2)\bar{c}_2 = 0 ,$$

and the first term of the strain's expansion at $\mathsf{x} = 0$ is $\bar{c}_0$; hence, from (109) and matching coefficients of the same order gives, for the first term,

$$\bar{c}_0 = -\delta^- + \delta_C + \mathsf{M}(T^- - T_C) . \qquad (128)$$

Therefore, the strain, strain gradient and the temperature at $\mathsf{z} = 0$ are related to the conditions at $\mathsf{z} \to -\infty$ by

$$\left. \begin{array}{l} \delta(0) - \delta^- = \bar{c}_0 + O(\varepsilon) , \\[2mm] \dot{\delta}(0) = \overset{+}{\beta}\bar{c}_0 + O(\varepsilon) , \\[2mm] T(0) - T^- = O(\varepsilon) , \end{array} \right\} \qquad (129)$$

where, for given (δ^-, T^-) and v, $\bar{c}_0$ is given by (128) and $\overset{\pm}{\beta}$ by (118). Observe that the strain gradient is given here with respect to the inner coordinate.

In view of the above, the composite expansion for the low strain phase is

$$\delta(z) - \delta^- = \bar{c}_0 e^{\overset{+}{\beta}z/\varepsilon} + O(\varepsilon) \quad \text{for } z < 0 \ .$$

Therefore, for given (δ^-, T^-) and v, the composite expansion for the low strain phase is completely determined up to $O(\varepsilon)$.

High strain phase.

For the inner solution close to $z = b$, since $\overset{+}{\beta} > 0$, the exponential term with exponent $\overset{+}{\beta}x$ is discarded. Hence, the inner solution is

$$\delta(x) - \delta^+ = \bar{\phi}_0(x) + O(\varepsilon) \ ,$$

where $\bar{\phi}_0(x) = \bar{c}_1 e^{\overline{\beta}(x - \bar{b})} + \bar{c}_2$ and $\bar{b} = b/\varepsilon$. The boundary condition (111) at $x = \bar{b}$ relates the strain and the temperature. From (127), expressed for the high strain phase, it follows that the lowest order term of the temperature's expansion at $x = \bar{b}$ is

$$\frac{1}{\mathsf{G}} \left[(1 - v^2)\bar{\phi}_0(\bar{b}) - \omega v \dot{\bar{\phi}}_0(\bar{b}) - \ddot{\bar{\phi}}_0(\bar{b}) \right] = \frac{1}{\mathsf{G}}(1 - v^2)\bar{c}_2 \ . \qquad (130)$$

The first term of the strain's expansion at $x = \bar{b}$ is $\bar{c}_1 + \bar{c}_2$, hence, using (130), the lowest order term in (111) gives

$$\bar{c}_1 + \bar{c}_2 - (\delta_C - \delta^+) = \mathsf{m} \left[\frac{1}{\mathsf{G}}(1 - v^2)\bar{c}_2 - (T_C - T^+) \right] \ . \qquad (131)$$

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Therefore, the strain, strain gradient and the temperature at $x = \bar{b}$ are related to the conditions at $z \to +\infty$ by

$$
\left.
\begin{aligned}
\delta(\bar{b}) - \delta^+ &= \bar{c}_1 + \bar{c}_2 + O(\varepsilon) \ , \\
\dot{\delta}(\bar{b}) &= \bar{\beta}\bar{c}_1 + O(\varepsilon) \ , \\
T(\bar{b}) - T^+ &= \frac{1}{G}(1 - v^2)\bar{c}_2 + O(\varepsilon) \ .
\end{aligned}
\right\}
\tag{132}
$$

In this case, the outer solution is nontrivial and the first term is given by (116). For the high strain phase it is convenient to work with $z - b$ instead of z. The translation is absorbed by the integration constant c_0. The outer expansion, rewritten in inner variables and expanded for small ε (with x fixed) gives

$$
\frac{r_2}{r_2 c_0 - r_0} + \dots \ ,
$$

where $r_2 = r_2(v, T^+)$. The inner expansion rewritten in outer coordinates, expanded for small ε (with z fixed) and rewritten in inner coordinates gives $\bar{c}_2 + \dots$; hence, for the inner and outer expansion to match asymptotically, it is necessary that

$$
\bar{c}_2 = \frac{r_2}{r_2 c_0 - r_0} \ .
\tag{133}
$$

The one-term composite expansion is obtained by adding the one-term inner and outer expansions and subtracting the one-term outer expansion of the one-term inner expansion, i.e.,

$$
\delta(z) - \delta^+ = \frac{r_2}{r_2 c_0 e^{-r_2(z-b)} - r_0} + \bar{c}_1 e^{\bar{\beta}(z-b)/\varepsilon} + O(\varepsilon) \ .
$$

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The temperature in the high strain phase is, from (117), (127) and the above expression for the strain, given by

$$T(z) - T^+ = \frac{1}{G}(1 - v^2)\left[\frac{r_2}{r_2 c_0 e^{-r_2(z-b)} - r_0}\right] + O(\varepsilon) \ .$$

Notice that the *inner* expansion of the temperature is, up to $O(\varepsilon)$, a *constant* given by $(1/G)(1 - v^2)\bar{c}_2$.

Unstable phase.

Since $T_0 = T(0^-) = T^- + O(\varepsilon)$, then, from (122) and enforcing the continuity of the strain, strain gradient and temperature at $x = 0$, it follows that

$$\left.\begin{aligned}
\bar{c}_1^u + \bar{c}_2^u - \frac{k_2}{k_1} &= \bar{c}_0 \ , \\
\bar{c}_1^u \overset{+}{\beta}_u + \bar{c}_2^u \overset{-}{\beta}_u &= \overset{+}{\beta}\bar{c}_0 \ .
\end{aligned}\right\}$$

Let

$$\delta_u = \delta^- - \frac{k_2}{k_1} \ , \tag{134}$$

and set $\delta_M = \delta_M(T^-)$ and $\delta_m = \delta_m(T^-)$; using the identities

$$\bar{c}_0 = \delta_M - \delta^- \ , \qquad \frac{\delta_M - \delta_u}{\delta_M - \delta^-} = \frac{\overset{+}{\beta}\overset{-}{\beta}}{\overset{+}{\beta}_u\overset{-}{\beta}_u} \ ,$$

it follows that

$$\bar{c}_1^u = \frac{1}{Q}\left[\frac{\bar{\beta}_u}{\bar{\beta}}(\overset{+}{\beta}_u - \bar{\beta})\right](\delta_M - \delta_u) \, , \\
\bar{c}_2^u = -\frac{1}{Q}\left[\frac{\overset{+}{\beta}_u}{\bar{\beta}}(\bar{\beta}_u - \bar{\beta})\right](\delta_M - \delta_u) \, , \Bigg\} \tag{135}$$

where $Q = Q(\mathsf{v}, T^-)$ is given by (124), $\bar{\beta}$ by (118), δ_u by (134) and (121) and $\overset{\pm}{\beta}_u$ by (123). The phase segregation condition at $\mathsf{x} = \bar{\mathsf{b}}$ specifies that the material is on the interface between the unstable and the high strain phase. Since the temperature throughout the unstable phase is essentially constant (up to $O(\varepsilon)$) then, from (122) and up to the leading term, this condition corresponds to

$$\bar{c}_1^u e^{\overset{+}{\beta}_u \bar{\mathsf{b}}} + \bar{c}_2^u e^{\bar{\beta}_u \bar{\mathsf{b}}} = \delta_m - \delta_u \, . \tag{136}$$

Now, enforcing continuity of temperature at $\mathsf{x} = \bar{\mathsf{b}}$, gives, from (132)$_3$,

$$\bar{c}_2 = \frac{\mathsf{G}}{1 - \mathsf{v}^2}(T^- - T^+) \, .$$

Using the above expression in (131), the constant $\bar{c}_1$ becomes

$$\bar{c}_1 = \delta_C - \delta^+ + \mathsf{m}(T^- - T_C) - \frac{\mathsf{G}}{1 - \mathsf{v}^2}(T^- - T^+) \, .$$

Let

$$\delta_*^+ = \frac{1}{1 - \mathsf{v}^2} + \delta^- \, . \tag{137}$$

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This quantity can be thought of as the strain (in the high strain phase) corresponding to the front state (δ_*^+, T^-) of an *isothermal* phase boundary for a given back state (δ^-, T^-). The state (δ_*^+, T^-) can also be viewed as the back state of an *adiabatic* shock wave for a given front state (δ^-, T^-). It is important to notice that the strain gradient at (δ_*^+, T^-) does not vanish, hence this state is not an equilibrium point of the system (110). Using $(36)_1$ and (137), the constants $\bar{c}_{1,2}$ can be expressed as $\bar{c}_1 = \delta_m - \delta_*^+$ and $\bar{c}_2 = \delta_*^+ - \delta^+$. The boundary condition (111) was used to determine the asymptotic expansion in the high strain phase and (136) was obtained by enforcing the phase segregation condition for the asymptotic expansion in the unstable phase. Therefore, the continuity of the strain at $x = \bar{b}$ is automatically satisfied from the continuity of the temperature. The only remaining condition that has not been enforced is the continuity of the strain gradient at $x = \bar{b}$ (i.e., (107)). From the inner expansion for the strain in the high strain phase, it follows that

$$\dot{\delta}(\bar{b}^+) = \bar{\beta}\bar{c}_1 + O(\varepsilon) = \bar{\beta}(\delta_m - \delta_*^+) + O(\varepsilon) \ .$$

On the other hand, from the asymptotic expansion in the unstable phase, one has

$$\dot{\delta}(\bar{b}^-) = \overset{+}{\beta}_u \bar{c}_1^u e^{\overset{+}{\beta}_u \bar{b}} + \bar{\beta}_u \bar{c}_2^u e^{\bar{\beta}_u \bar{b}} + O(\varepsilon) \ ;$$

hence, up to the leading term, the closing condition for the construction of a traveling wave is

$$\overset{+}{\beta}_u \bar{c}_1^u e^{\overset{+}{\beta}_u \bar{b}} + \bar{\beta}_u \bar{c}_2^u e^{\bar{\beta}_u \bar{b}} = \bar{\beta}(\delta_m - \delta_*^+) \ . \tag{138}$$

It is possible to prove that

$$\frac{\delta_{\mathrm{m}} - \delta_u}{\delta_{\mathrm{m}} - \delta_*^+} = \frac{\overset{+}{\beta}\overset{-}{\beta}}{\overset{+}{\beta_u}\overset{-}{\beta_u}} \; .$$

In view of the above relation and using (124) and (135), equations (136) and (138) can be expressed, after some simplifications, as

$$e^{Q\bar{b}} = \left(\frac{P - Q}{P + Q}\right)^2 \; , \qquad (139)$$

and

$$e^{-v\omega\bar{b}} = \left(\frac{\overset{-}{\beta}}{\overset{+}{\beta}}\right)^2 \left(\frac{\delta_{\mathrm{m}} - \delta_u}{\delta_{\mathrm{M}} - \delta_u}\right)^2 \; . \qquad (140)$$

Since $\mathsf{v}^2 < 1$, then $P > 0$. Thus, if $Q > 0$, equation (139) has no solution since the left-hand side is always greater than the right-hand side for any $\bar{b} > 0$. Therefore, a necessary condition to obtain a solution is $Q = i|Q|$. Of all the possible roots of (139), only the smallest satisfies the phase segregation conditions, hence, choosing the argument of the complex number $P + i|Q|$ to be in the interval $(0, \pi/2)$, then, from (139),

$$\bar{b} = \frac{1}{|Q|} \left[2\pi - 4\arg(P + i|Q|)\right] \; . \qquad (141)$$

The width of the unstable region is therefore determined as a function of the velocity and the temperature T^-.

The *phase space* for the system of equations (108), (110) and (101) is

(δ, δ', T). Figure 3 shows the projection into the δ-T plane of the trajectory of a traveling wave such that $T^+ > T^-$ (in this case $\mathsf{v} = 0.05$). The Hugoniot curve $T = T^H(\delta)$, as defined in Section 2.3, is also shown. The corresponding wave profiles are shown in Figures 4 (inner coordinates) and 5 (outer coordinates). These graphs were obtained using the following values: $\mathsf{G} = 0.8$, $\mathsf{M} = 1.4$, $\mathsf{m} = 1.2$, $\delta_C = 3.1$, $T_T = 1$, $T_C = 3$, $l_T = 0.5$, $\omega = 1$ and $\varepsilon = 1/\varpi = 10^{-5}$. Similarly, Figures 6, 7 and 8 show a traveling wave such that $T^+ < T^-$ (in this case $\mathsf{v} = 0.7$). Observe that, in this case, the first portion of the wave, from δ^+ to δ_*^+, is *expansive*.

Kinetic relation.

As mentioned in Section 4.2, the values $(\delta^\pm, T^\pm, \mathsf{v})$ are formally related via the jump conditions $(36)_{1,2}$. If equation (141) is used to compute $\bar{\mathsf{b}}$, then (140) can be viewed as an *additional restriction* on the values of $(\delta^\pm, T^\pm, \mathsf{v})$. Hence, for a given pair of values (e.g., back state (δ^-, T^-) or front state (δ^+, T^+) or other combinations), the system $(36)_{1,2}$, (141) provides the necessary restrictions to determine the other three values (e.g., $(\delta^+, T^+, \mathsf{v})$, etc.). Notice that this relation only holds for $0 < \mathsf{v} < 1$ and, from the entropy inequality, it is also required that the driving traction should be positive. The condition (140) can also be interpreted in terms of the driving traction. To this end, the strain δ_u can be written, from (140), as

$$\delta_u = \delta_\mathsf{M} + \frac{\delta_\mathsf{m} - \delta_\mathsf{M}}{1 - (\overset{+}{\beta}/\overset{-}{\beta}) \exp[-\mathsf{v}\omega\bar{\mathsf{b}}/2]} \; .$$

Therefore, from (121), (134) and (137), the strains δ^- and δ_*^+ can be expressed as

$$\delta^- = \frac{1}{(1 - \mathsf{v}^2)} \left(\frac{\delta_u - \delta_M}{\delta_M - \delta_m} \right) + \delta_u \ ,$$

and

$$\delta_*^+ = \frac{1}{(1 - \mathsf{v}^2)} \left(\frac{\delta_u - \delta_m}{\delta_M - \delta_m} \right) + \delta_u \ .$$

Hence, formally, since $\bar{b}$ is a function of v and T^- and δ_m and δ_M are functions of T^-, then $\delta_u = \delta_u(\mathsf{v}, T^-)$ and $\delta^- = \delta^-(\mathsf{v}, T^-)$. Using this expression for δ^- in (37), the temperature T^+ can be obtained as a function of v and T^-. The strain δ^+ in the high strain phase can be determined from $(36)_1$. Finally, from (112), it is possible to obtain a kinetic relation of the form (29), i.e.,

$$\mathsf{f} = \mathsf{f}(\mathsf{v}, T^-) \ .$$

It is also possible to use T^+ as a reference temperature by solving for T^- and $\delta^\pm$ for given T^+ in which case $\mathsf{f} = \mathsf{f}(\mathsf{v}, T^+)$. Several kinetic curves, corresponding to different values of ω and a common value of $T^+ = 1.5$ are shown in Figure 9. The last point of each curve (for maximum v) corresponds to the limit $\delta^+ = \delta_m$ as required by the phase segregation condition $(97)_3$. All curves have a common value at $\mathsf{v} = 0$ (the parameter ω is always multiplied by v in the equations). Observe that for small enough values of ω, the corresponding kinetic curve is *non monotonic*. Relations of this kind have recently been considered by ROSAKIS & KNOWLES [23] in a purely mechanical context. It is interesting to point out that setting $\mathsf{v} = 0$ in (108), (110) and (120) results in $T(z)$ being constant, which is different from the limit $\mathsf{v} \to 0$ in the solution obtained by perturbation analysis. Moreover, the

energy jump condition $(36)_2$ and the entropy inequality $(36)_3$ are trivially satisfied when $v = 0$. Figure 10 shows a set of kinetic relations for different values of T^+ and a common value of $\omega = 1$. In this case, for a given velocity v, the driving traction decreases for increasing temperature T^+—the same behavior is observed when T^- is used as a reference temperature.

The negative velocity case is different than the positive one in the sense that $\overset{+}{\beta}$ and $\overset{-}{\beta}$ have the *same* sign. Even though it is possible to obtain a uniformly valid expansion for the low strain phase, there seems to be no simple way to construct such an expansion for the high strain phase.

An interesting point that arises from this analysis is that, although it is possible to formally cast the admissibility criterion in terms of a kinetic relation of the type proposed in [5], there is no simple dependence on the temperature. The temperature enters the kinetic relation in a somehow *arbitrary* way in the sense that either the temperature in front of a phase boundary or the temperature in the back can be used as a reference temperature. This fact was also observed by NGAN & TRUSKINOVSKY [20] in their numerical simulations and suggests that the functional form of the kinetic relation in the thermoelastic case should be reconsidered.

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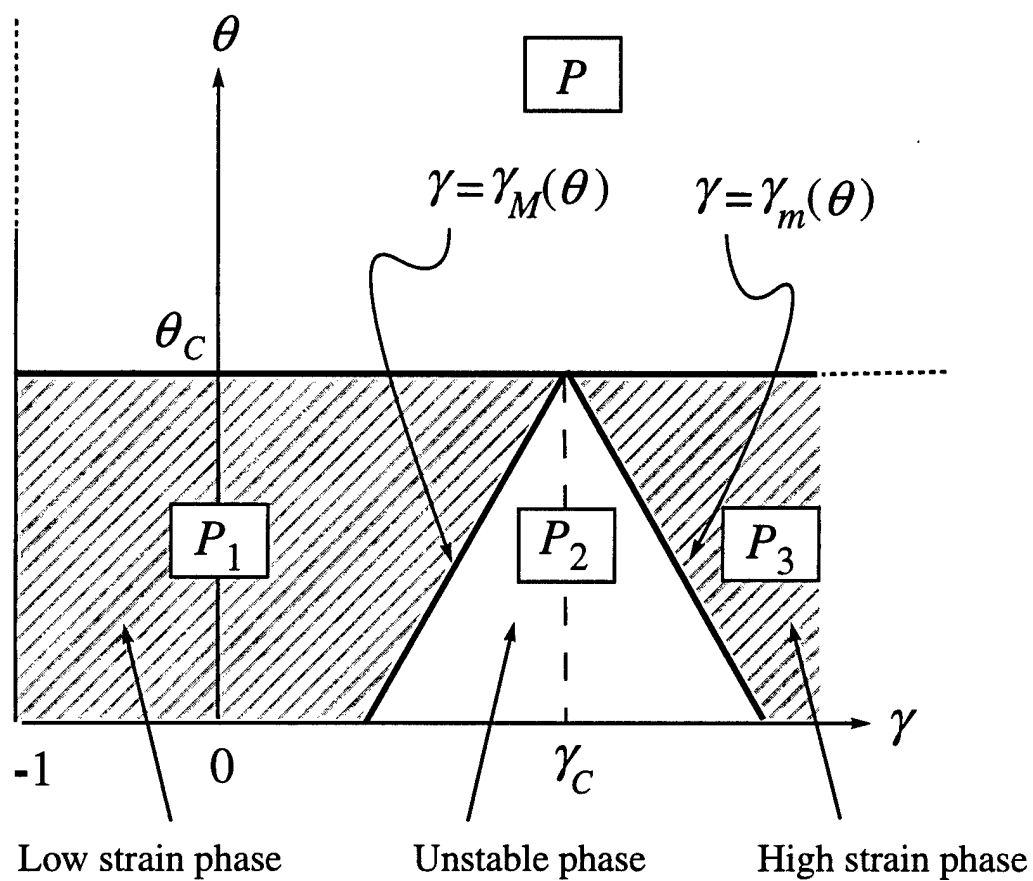
Figure 1: Material phases in the temperature-strain plane.
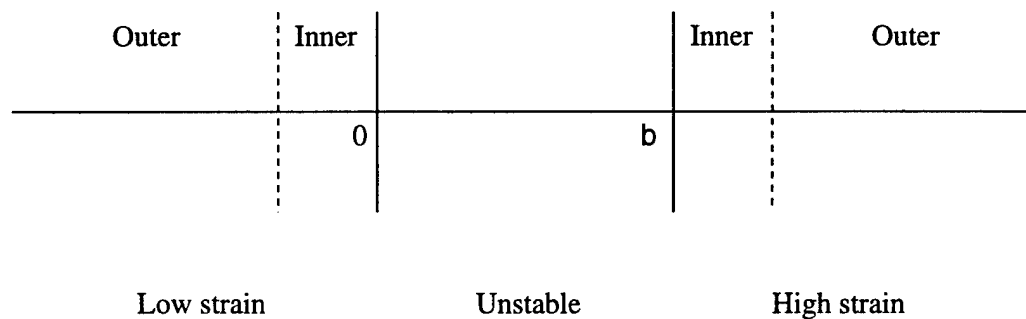
Figure 2: Outer and inner solutions for metastable phases.
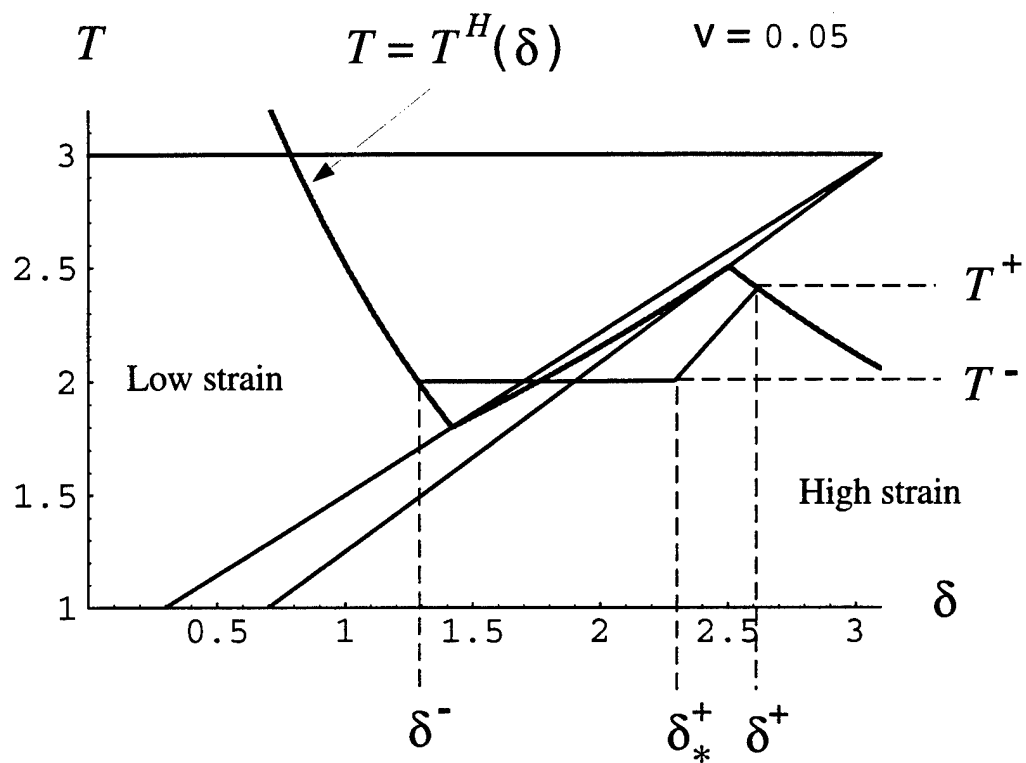
Figure 3: Projection of the trajectory of a traveling wave from the δ, δ', T-phase space into the δ, T-plane for $T^+ > T^-$. The Hugoniot curve $T = T^H(\delta)$ is based at (δ^+, T^+).
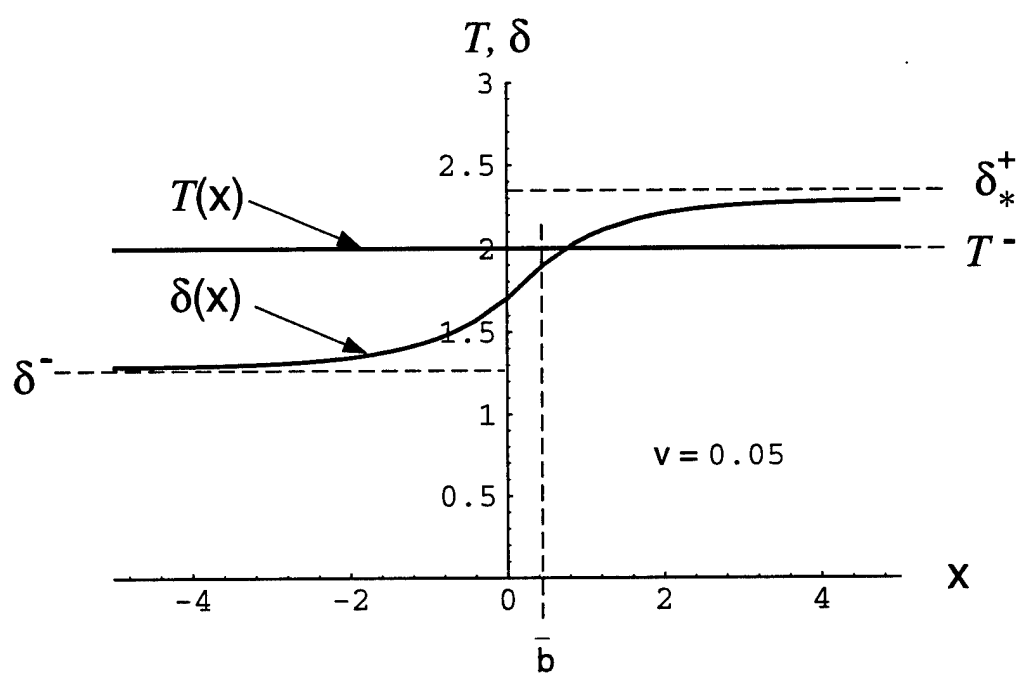
Figure 4: Strain and temperature wave profiles in inner coordinates for v = 0.05.
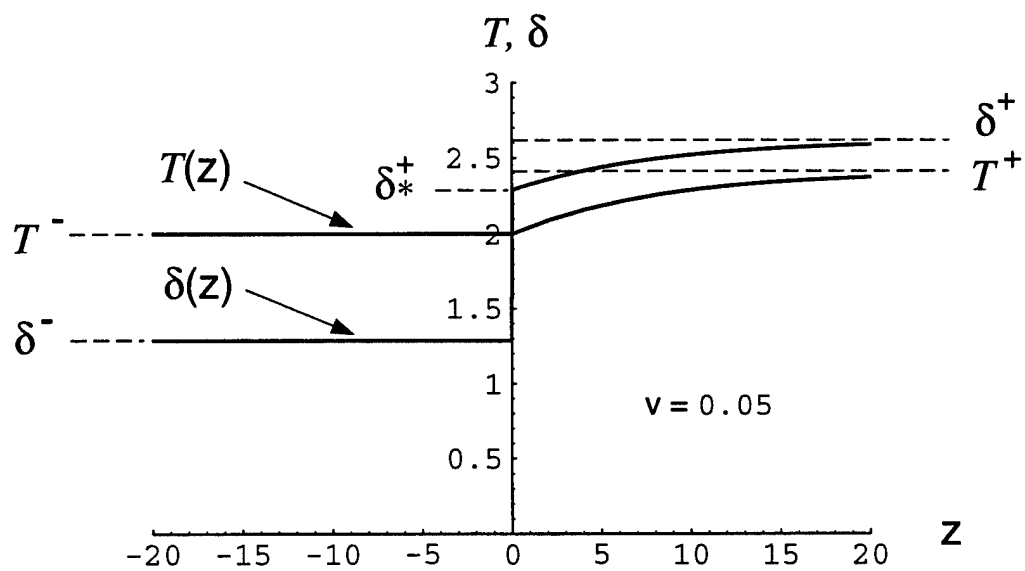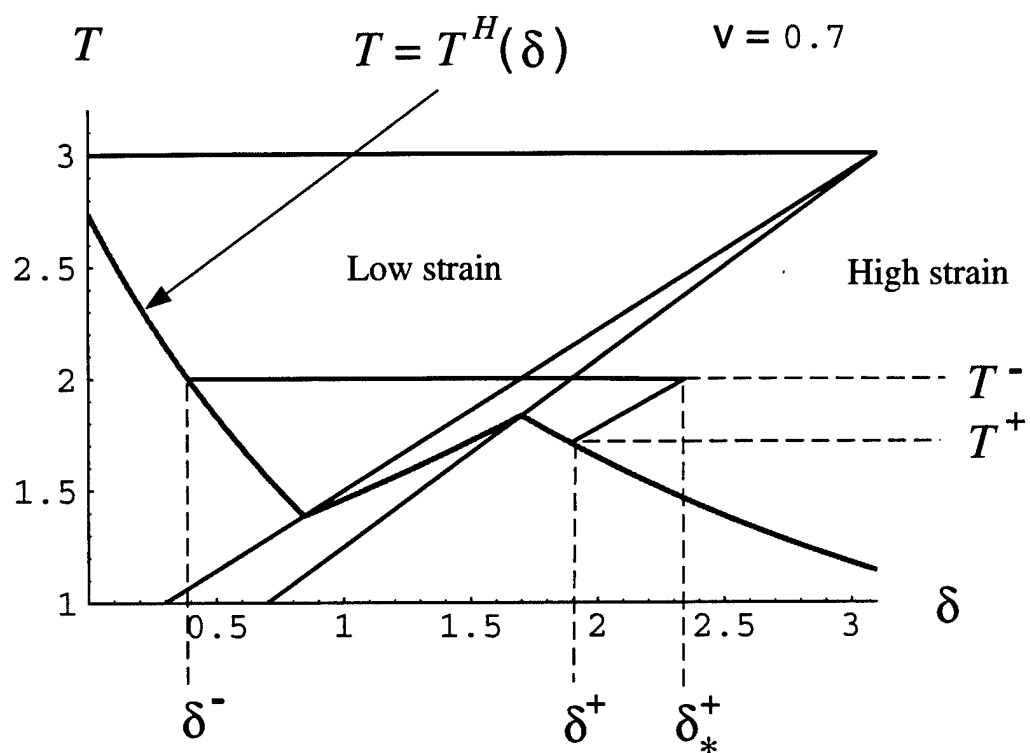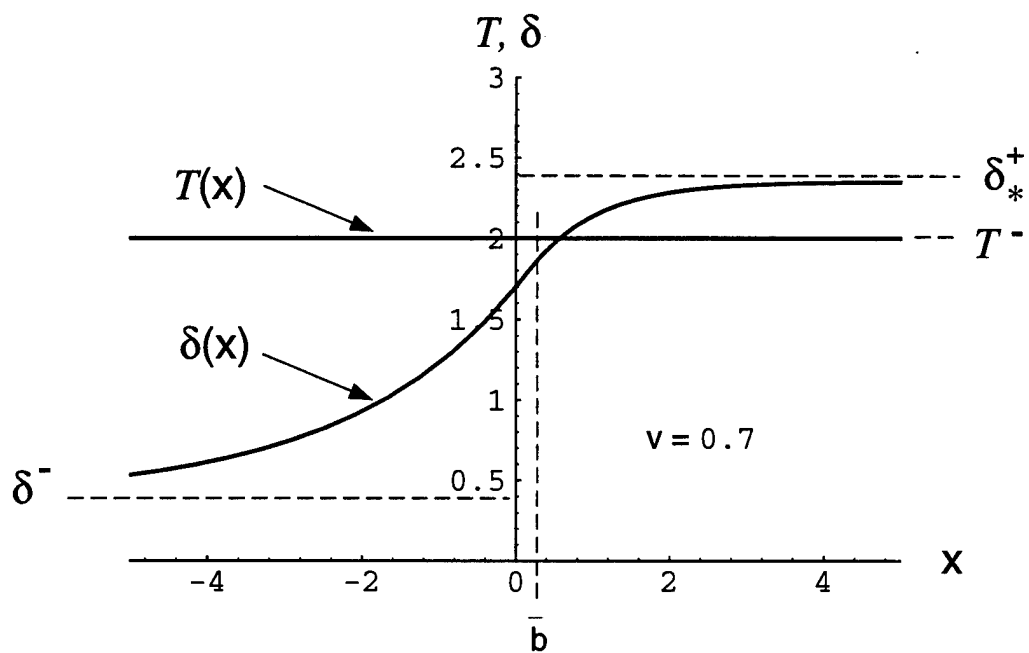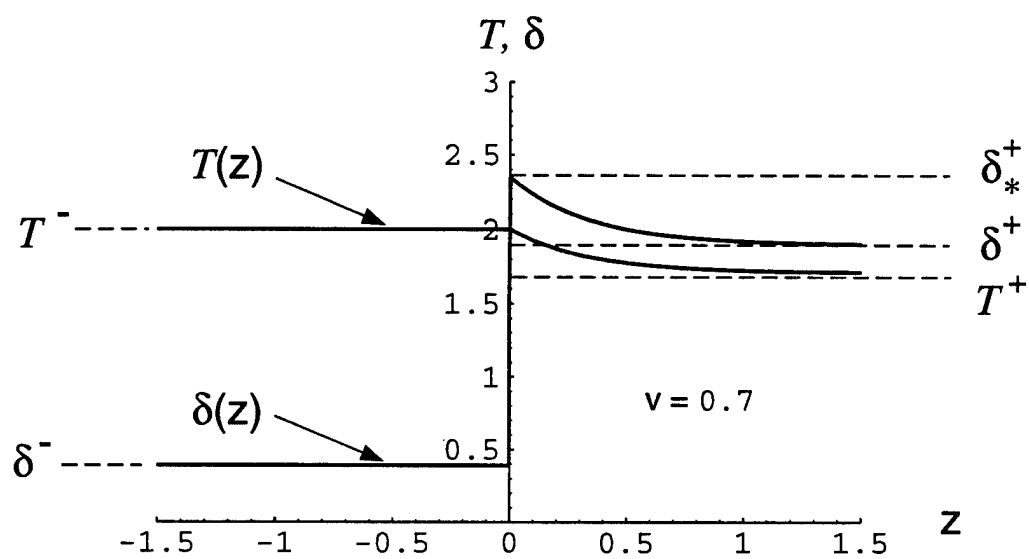
Figure 5: Strain and temperature wave profiles in outer coordinates for $v = 0.05$.

Figure 6: Projection of the trajectory of a traveling wave from the δ, δ', T-phase space into the δ, T-plane for $T^+ < T^-$. The Hugoniot curve $T = T^H(\delta)$ is based at (δ^+, T^+).

Figure 7: Strain and temperature wave profiles in inner coordinates for $v = 0.7$.

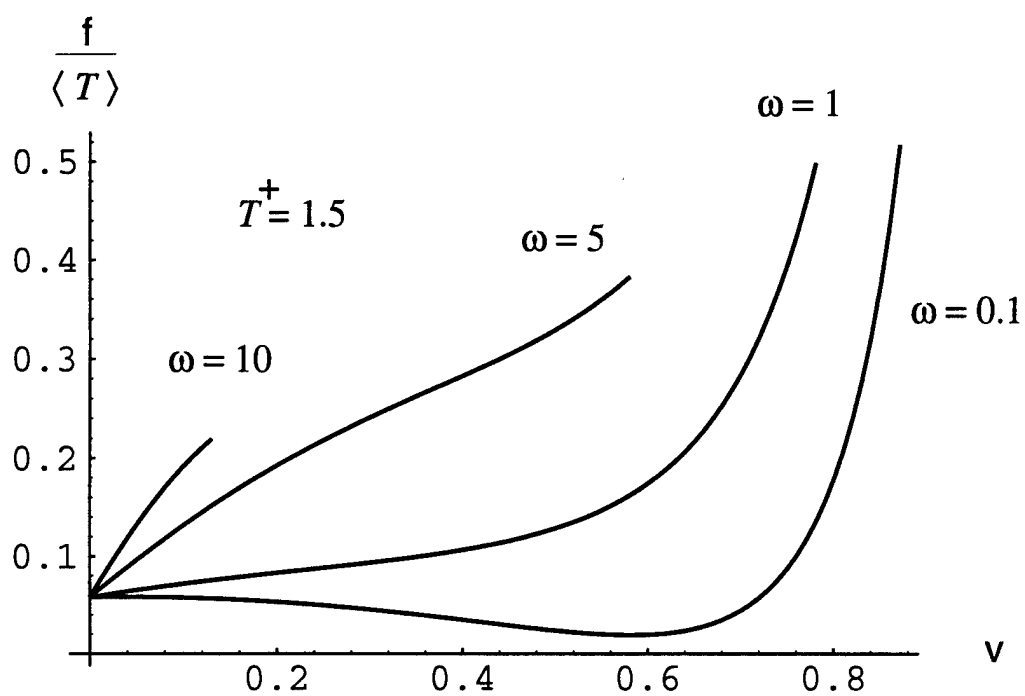Figure 8: Strain and temperature wave profiles in outer coordinates for v = 0.7.

Figure 9: Kinetic curves for front state temperature $T^+ = 1.5$ and various values of the material parameter ω.
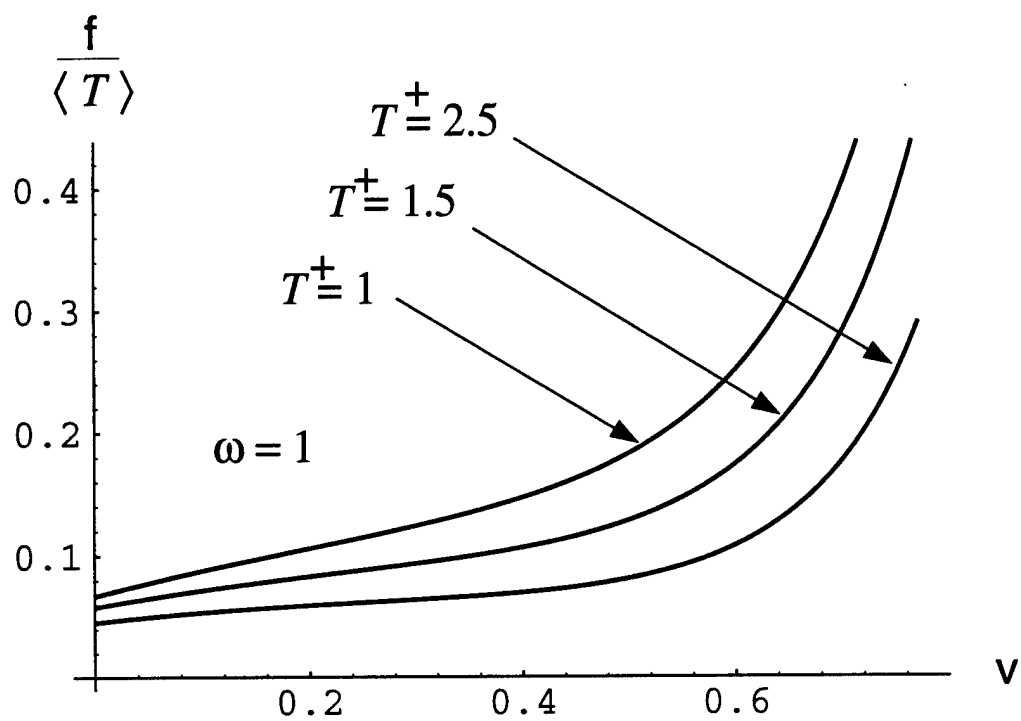
Figure 10: Kinetic curves for the material parameter $\omega = 1$ and various values of the front state temperature T^+.

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The theory of thermoelastic materials undergoing solid-solid phase transformations requires constitutive information that governs the evolution of a phase boundary. This is known as a kinetic relation which relates a driving traction to the speed of propagation of a phase boundary. The kinetic relation is prescribed in the theory from the onset. Here, though, a special kinetic relation is derived from an augmented theory that includes viscous, strain gradient and heat conduction effects. Based on a special class of solutions, namely traveling waves, the kinetic relation is inherited from the augmented theory as the viscosity, strain gradient and heat conductivity are removed by a suitable limit process.

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